



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:37 AM UTC

PDB ID : 9GAI / pdb_00009gai
Title : 3-methylbenzoyl-CoA reductase from Thauera chlorobenzoica (MbdONPQ)
Authors : Ermler, U.; Boll, M.; Demmer, U.; Fuchs, J.
Deposited on : 2024-07-29
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

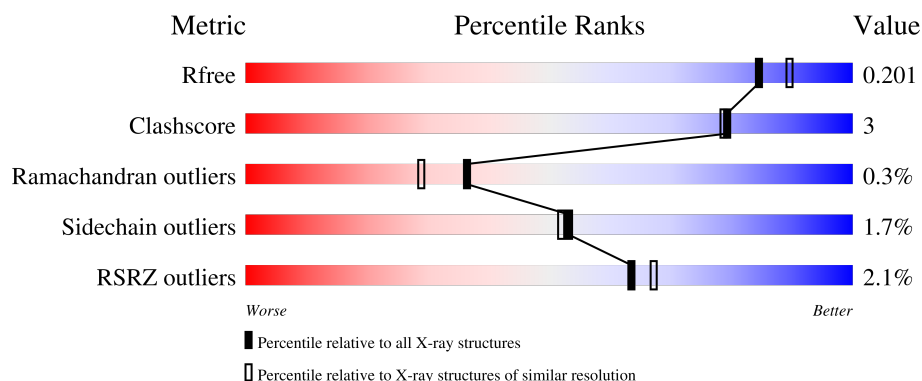
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



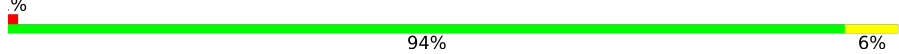
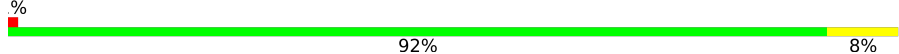
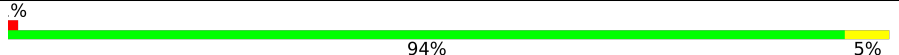
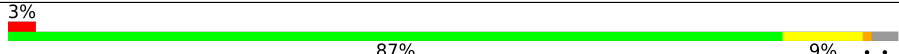
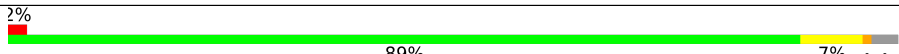
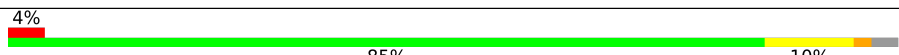
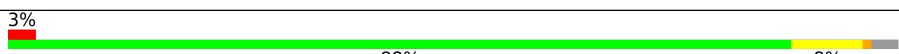
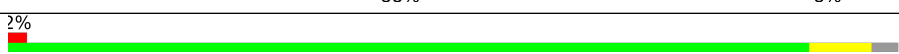
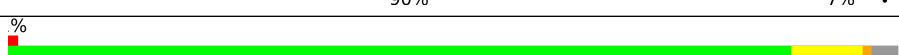
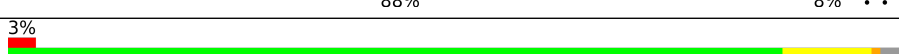
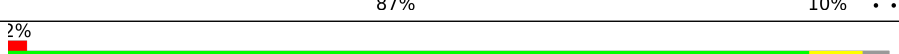
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	445	<div> <div>3%</div> <div>90%</div> <div>7%</div> <div>..</div> </div>
1	E	445	<div> <div>2%</div> <div>91%</div> <div>7%</div> <div>.</div> </div>
1	I	445	<div> <div>2%</div> <div>91%</div> <div>7%</div> <div>.</div> </div>
1	M	445	<div> <div>3%</div> <div>93%</div> <div>6%</div> <div>.</div> </div>
2	B	388	<div> <div>%</div> <div>93%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain	
2	F	388		%
2	J	388		%
2	N	388		%
3	C	273		%
3	G	273		%
3	K	273		%
3	O	273		%
4	D	269		%
4	H	269		%
4	L	269		%
4	P	269		%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	GOL	N	403	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 45019 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 3-methylbenzoyl-CoA reductase beta subunit MbdO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	6	0
			3508	2224	611	655	18			
1	E	436	Total	C	N	O	S	0	3	0
			3475	2202	602	653	18			
1	I	437	Total	C	N	O	S	0	2	0
			3472	2201	601	652	18			
1	M	437	Total	C	N	O	S	0	3	0
			3476	2203	601	653	19			

- Molecule 2 is a protein called 3-methylbenzoyl-CoA reductase gamma subunit MbdN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	387	Total	C	N	O	S	0	4	0
			3127	1983	532	597	15			
2	F	387	Total	C	N	O	S	0	2	0
			3110	1974	528	593	15			
2	J	387	Total	C	N	O	S	0	1	0
			3099	1968	526	590	15			
2	N	387	Total	C	N	O	S	0	4	0
			3128	1984	534	595	15			

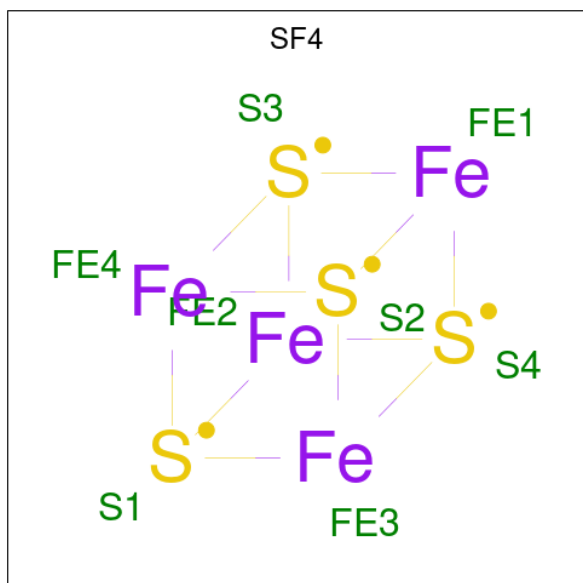
- Molecule 3 is a protein called 3-methylbenzoyl-CoA reductase delta subunit MbdP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	264	Total	C	N	O	S	0	3	0
			2023	1264	360	385	14			
3	G	264	Total	C	N	O	S	0	3	0
			2026	1266	363	383	14			
3	K	264	Total	C	N	O	S	0	6	0
			2054	1281	369	390	14			
3	O	265	Total	C	N	O	S	0	3	0
			2027	1266	361	386	14			

- Molecule 4 is a protein called 3-methylbenzoyl-CoA reductase alpha subunit MbdQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	261	Total	C	N	O	S	0	4	0
			1963	1232	354	366	11			
4	H	261	Total	C	N	O	S	0	2	0
			1945	1221	349	364	11			
4	L	261	Total	C	N	O	S	0	3	0
			1948	1224	347	365	12			
4	P	261	Total	C	N	O	S	0	1	0
			1934	1215	345	363	11			

- Molecule 5 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			8	4	4		
5	B	1	Total	Fe	S	0	0
			8	4	4		
5	C	1	Total	Fe	S	0	0
			8	4	4		
5	E	1	Total	Fe	S	0	0
			8	4	4		
5	F	1	Total	Fe	S	0	0
			8	4	4		
5	G	1	Total	Fe	S	0	0
			8	4	4		

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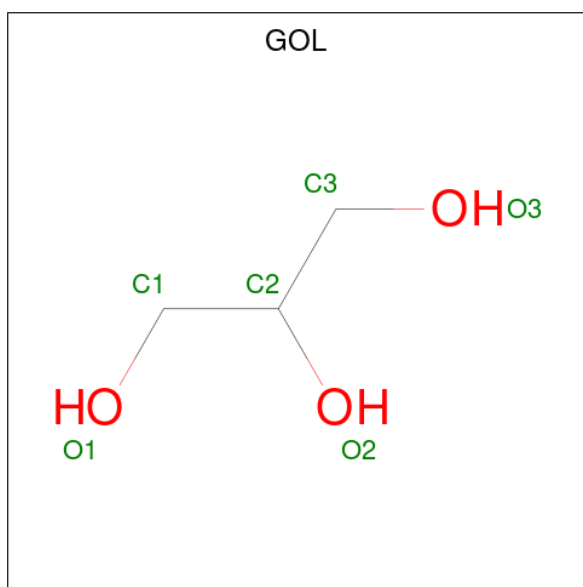
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	I	1	Total	Fe	S	0	0
			8	4	4		
5	J	1	Total	Fe	S	0	0
			8	4	4		
5	K	1	Total	Fe	S	0	0
			8	4	4		
5	M	1	Total	Fe	S	0	0
			8	4	4		
5	N	1	Total	Fe	S	0	0
			8	4	4		
5	O	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		
6	E	1	Total	Cl	0	0
			1	1		
6	F	1	Total	Cl	0	0
			1	1		
6	I	1	Total	Cl	0	0
			1	1		
6	J	1	Total	Cl	0	0
			1	1		
6	M	1	Total	Cl	0	0
			1	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	I	1	Total	C	O	0	0
			6	3	3		
7	I	1	Total	C	O	0	0
			6	3	3		
7	M	1	Total	C	O	0	0
			6	3	3		
7	M	1	Total	C	O	0	0
			6	3	3		
7	N	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	K	0	0
			1	1		
8	B	1	Total	K	0	0
			1	1		

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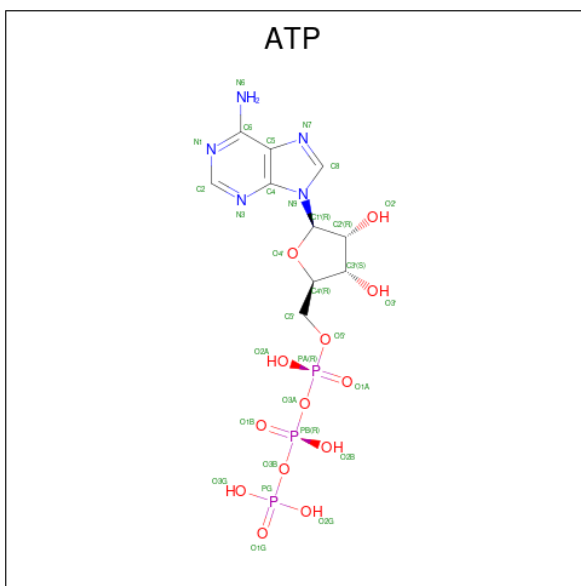
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	F	1	Total K 1 1	0	0
8	J	3	Total K 3 3	0	0
8	N	1	Total K 1 1	0	0
8	O	1	Total K 1 1	0	0
8	P	1	Total K 1 1	0	0

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Mg 1 1	0	0
9	C	1	Total Mg 1 1	0	0
9	D	1	Total Mg 1 1	0	0
9	E	1	Total Mg 1 1	0	0
9	F	1	Total Mg 1 1	0	0
9	G	1	Total Mg 1 1	0	0
9	H	2	Total Mg 2 2	0	0
9	K	1	Total Mg 1 1	0	0
9	L	2	Total Mg 2 2	0	0
9	M	1	Total Mg 1 1	0	0
9	N	1	Total Mg 1 1	0	0
9	O	1	Total Mg 1 1	0	0
9	P	1	Total Mg 1 1	0	0

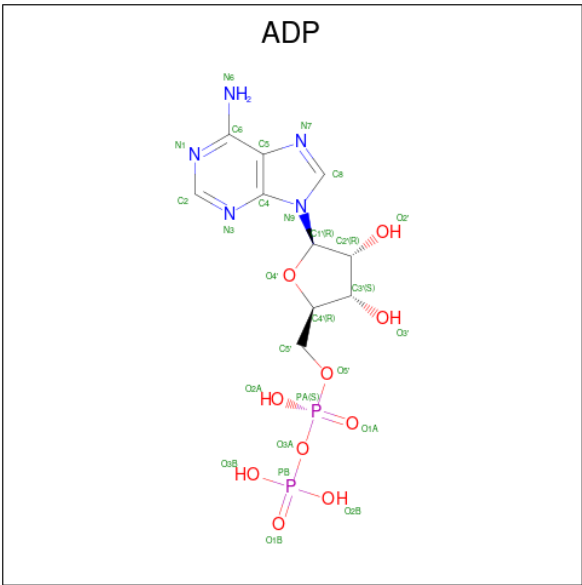
- Molecule 10 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃)

(labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
10	G	1	Total 31	C 10	N 5	O 13	P 3	0	0
10	K	1	Total 31	C 10	N 5	O 13	P 3	0	0
10	O	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
11	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
11	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
11	P	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	191	Total	O	0	1
			192	192		
12	B	182	Total	O	0	1
			183	183		
12	C	91	Total	O	0	0
			91	91		
12	D	62	Total	O	0	1
			63	63		
12	E	183	Total	O	0	2
			185	185		
12	F	168	Total	O	0	0
			168	168		
12	G	103	Total	O	0	0
			103	103		
12	H	92	Total	O	0	1
			93	93		

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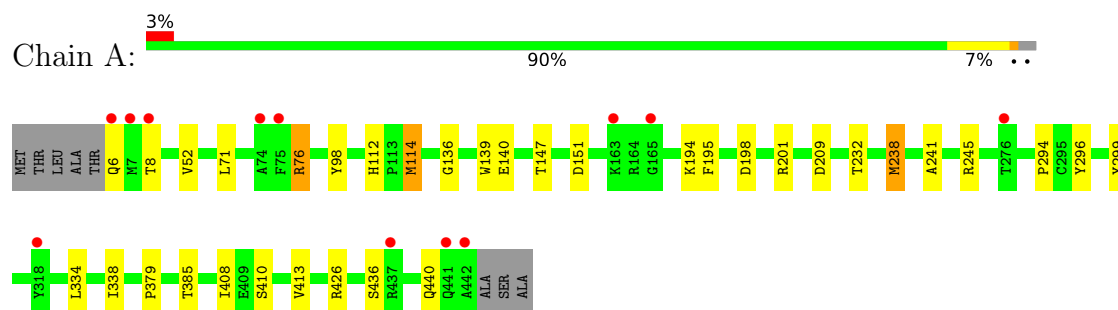
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	I	194	Total 195	O 195	0	1
12	J	190	Total 190	O 190	0	0
12	K	73	Total 73	O 73	0	0
12	L	73	Total 73	O 73	0	0
12	M	201	Total 202	O 202	0	1
12	N	278	Total 279	O 279	0	1
12	O	107	Total 107	O 107	0	0
12	P	88	Total 89	O 89	0	1

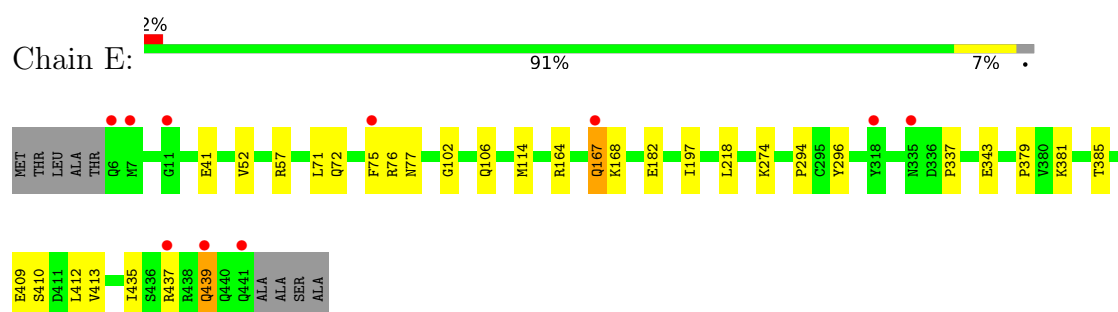
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

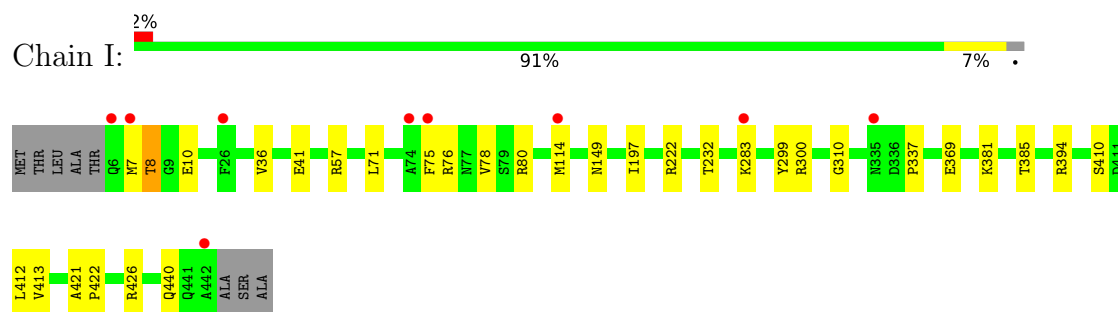
- Molecule 1: 3-methylbenzoyl-CoA reductase beta subunit MbdO



- Molecule 1: 3-methylbenzoyl-CoA reductase beta subunit MbdO

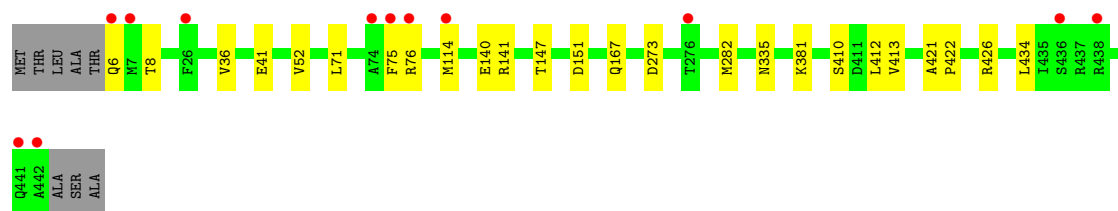


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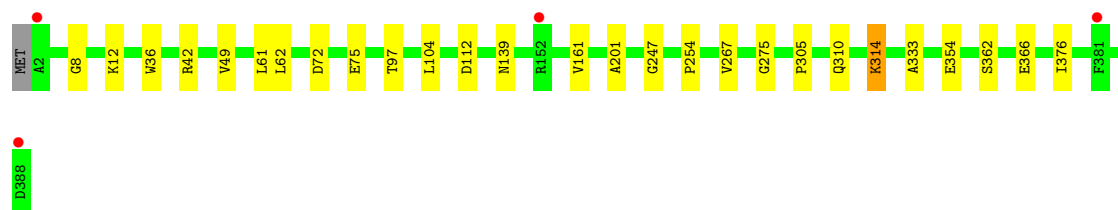


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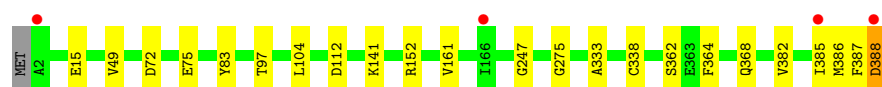




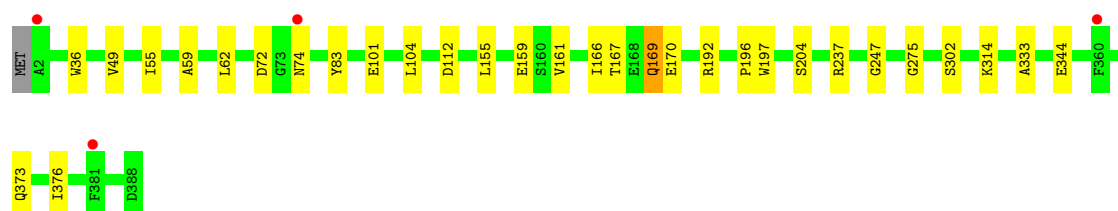
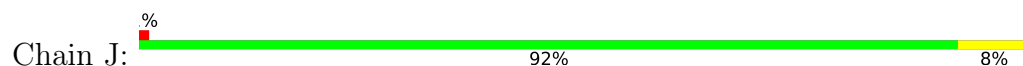
- Molecule 2: 3-methylbenzoyl-CoA reductase gamma subunit MbdN



- Molecule 2: 3-methylbenzoyl-CoA reductase gamma subunit MbdN



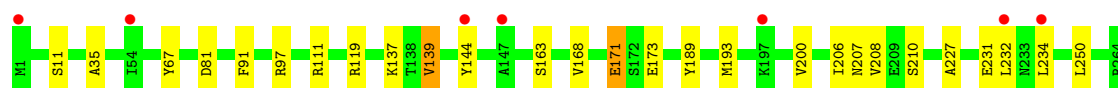
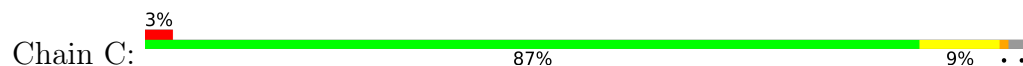
- Molecule 2: 3-methylbenzoyl-CoA reductase gamma subunit MbdN



- Molecule 2: 3-methylbenzoyl-CoA reductase gamma subunit MbdN

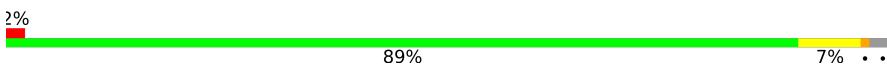


- Molecule 3: 3-methylbenzoyl-CoA reductase delta subunit MbdP




GLY
SER
GLY
GLY
ASP
ARG
ARG
ALA
ALA

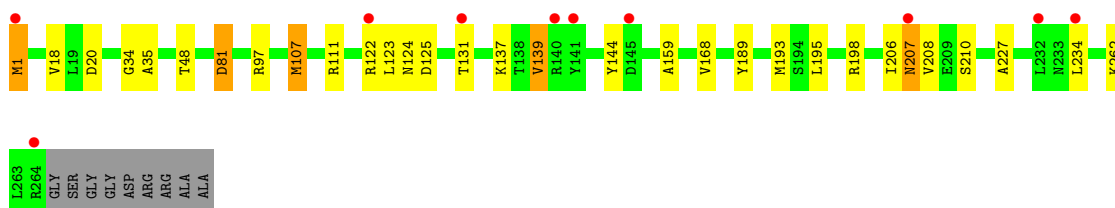
- Molecule 3: 3-methylbenzoyl-CoA reductase delta subunit MbdP

Chain G:  2% 89% 7% . .




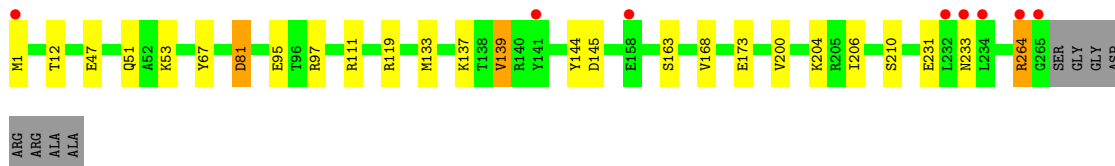
- Molecule 3: 3-methylbenzoyl-CoA reductase delta subunit MbdP

Chain K:  4% 85% 10% . .



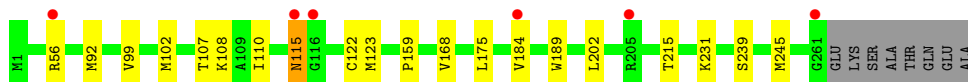
- Molecule 3: 3-methylbenzoyl-CoA reductase delta subunit MbdP

Chain O:  3% 88% 8% . .

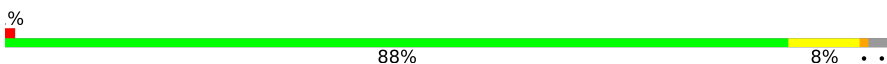


- Molecule 4: 3-methylbenzoyl-CoA reductase alpha subunit MbdQ

Chain D:  2% 90% 7% .




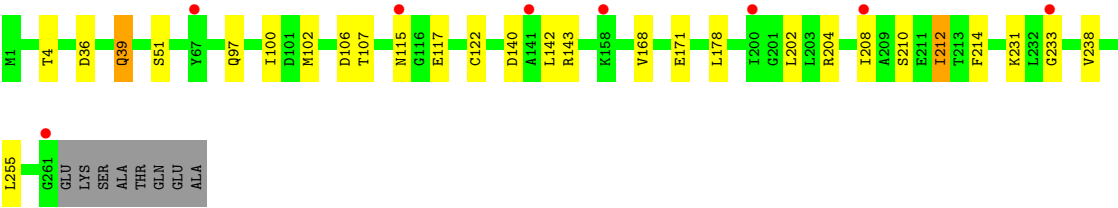
- Molecule 4: 3-methylbenzoyl-CoA reductase alpha subunit MbdQ

Chain H:  0% 88% 8% . .

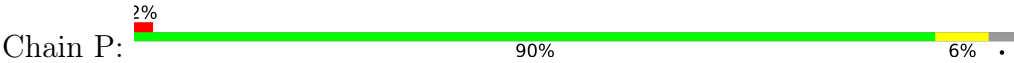


- Molecule 4: 3-methylbenzoyl-CoA reductase alpha subunit MbdQ

Chain L:  3% 87% 10% . .



● Molecule 4: 3-methylbenzoyl-CoA reductase alpha subunit MbdQ



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	146.52Å 203.16Å 235.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.66 – 1.90 48.66 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.66-1.90) 99.9 (48.66-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.174 , 0.201 0.174 , 0.201	Depositor DCC
R_{free} test set	27140 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	45019	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SF4, ADP, CL, K, ATP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.32	0/3583	0.51	0/4839
1	E	0.33	0/3550	0.51	0/4797
1	I	0.33	0/3547	0.52	0/4793
1	M	0.34	0/3551	0.51	0/4799
2	B	0.30	0/3193	0.48	0/4326
2	F	0.29	0/3176	0.48	0/4304
2	J	0.31	0/3165	0.49	0/4289
2	N	0.37	0/3194	0.54	0/4328
3	C	0.32	0/2050	0.51	0/2765
3	G	0.31	0/2053	0.50	0/2768
3	K	0.26	0/2081	0.45	0/2805
3	O	0.32	0/2054	0.52	0/2770
4	D	0.26	0/1991	0.44	0/2680
4	H	0.31	0/1973	0.49	0/2656
4	L	0.27	0/1976	0.46	0/2661
4	P	0.29	0/1962	0.48	0/2642
All	All	0.31	0/43099	0.50	0/58222

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3508	0	3450	21	0
1	E	3475	0	3404	18	0
1	I	3472	0	3404	22	0
1	M	3476	0	3405	13	0
2	B	3127	0	3060	16	0
2	F	3110	0	3046	14	0
2	J	3099	0	3040	21	0
2	N	3128	0	3066	16	0
3	C	2023	0	2047	16	0
3	G	2026	0	2056	13	0
3	K	2054	0	2076	21	0
3	O	2027	0	2050	14	0
4	D	1963	0	1998	14	0
4	H	1945	0	1978	13	0
4	L	1948	0	1980	16	0
4	P	1934	0	1966	9	0
5	A	8	0	0	0	0
5	B	8	0	0	0	0
5	C	8	0	0	0	0
5	E	8	0	0	0	0
5	F	8	0	0	1	0
5	G	8	0	0	0	0
5	I	8	0	0	0	0
5	J	8	0	0	0	0
5	K	8	0	0	0	0
5	M	8	0	0	0	0
5	N	8	0	0	0	0
5	O	8	0	0	0	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	M	1	0	0	0	0
7	A	18	0	23	2	0
7	E	12	0	16	0	0
7	I	12	0	16	0	0
7	M	12	0	16	0	0
7	N	6	0	7	5	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	F	1	0	0	0	0
8	J	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	N	1	0	0	0	0
8	O	1	0	0	0	0
8	P	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
9	G	1	0	0	0	0
9	H	2	0	0	0	0
9	K	1	0	0	0	0
9	L	2	0	0	0	0
9	M	1	0	0	0	0
9	N	1	0	0	0	0
9	O	1	0	0	0	0
9	P	1	0	0	0	0
10	C	31	0	12	0	0
10	G	31	0	12	0	0
10	K	31	0	12	0	0
10	O	31	0	12	0	0
11	D	27	0	12	0	0
11	H	27	0	12	0	0
11	L	27	0	12	0	0
11	P	27	0	12	0	0
12	A	192	0	0	5	0
12	B	183	0	0	1	0
12	C	91	0	0	0	0
12	D	63	0	0	0	0
12	E	185	0	0	2	0
12	F	168	0	0	1	0
12	G	103	0	0	0	0
12	H	93	0	0	1	0
12	I	195	0	0	6	0
12	J	190	0	0	1	0
12	K	73	0	0	0	0
12	L	73	0	0	0	0
12	M	202	0	0	2	0
12	N	279	0	0	1	0
12	O	107	0	0	1	0
12	P	89	0	0	0	0
All	All	45019	0	42200	232	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 3.

All (232) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:208:ILE:HG23	4:L:212:ILE:HD11	1.53	0.88
1:I:7:MET:HE3	1:I:8:THR:H	1.46	0.81
2:N:169:GLN:HB2	7:N:403:GOL:H12	1.64	0.80
3:K:111:ARG:HG2	3:K:206:ILE:HD12	1.70	0.73
1:I:76[B]:ARG:HG2	1:I:114:MET:HE3	1.72	0.71
2:J:59:ALA:HB2	2:J:166:ILE:HD11	1.73	0.69
3:C:208:VAL:HG21	3:C:234:LEU:HD13	1.73	0.69
3:G:14:ILE:HG13	3:G:33:THR:HG22	1.73	0.69
1:I:197:ILE:HD11	1:I:337:PRO:HG2	1.74	0.68
1:E:379:PRO:HG2	1:E:409:GLU:HG2	1.75	0.68
3:C:111:ARG:HG2	3:C:206:ILE:HD12	1.75	0.68
1:A:198:ASP:OD1	1:A:201[A]:ARG:NH2	2.27	0.67
1:A:294:PRO:HG2	1:A:296:TYR:CZ	2.32	0.65
1:E:197:ILE:HD11	1:E:337:PRO:HG2	1.78	0.65
1:I:76[A]:ARG:HG2	1:I:114:MET:HE3	1.78	0.64
4:L:233:GLY:HA3	2:N:16:GLN:HG3	1.79	0.64
2:F:247:GLY:HA3	2:F:333:ALA:O	1.96	0.64
3:K:208:VAL:HG21	3:K:234:LEU:HD13	1.79	0.64
1:E:41:GLU:HG2	3:O:95:GLU:HG3	1.81	0.63
4:D:108:LYS:HG2	4:D:123:MET:HG2	1.80	0.63
1:M:167:GLN:NE2	12:M:601:HOH:O	2.31	0.63
2:J:159:GLU:HG2	2:J:166:ILE:HD12	1.81	0.62
4:L:36:ASP:CG	4:L:39:GLN:HB2	2.25	0.61
1:M:76:ARG:HH11	1:M:76:ARG:HB3	1.65	0.61
3:K:35:ALA:HB2	4:L:142:LEU:HA	1.84	0.59
4:H:115:ASN:N	4:H:115:ASN:OD1	2.34	0.59
4:H:108:LYS:HG2	4:H:123:MET:HG2	1.86	0.58
3:C:200:VAL:HG11	3:C:231:GLU:HG3	1.85	0.58
3:C:97[B]:ARG:HD2	3:C:210:SER:O	2.04	0.58
1:E:294:PRO:HG2	1:E:296:TYR:CZ	2.40	0.57
1:E:435:ILE:O	1:E:439:GLN:HG2	2.04	0.57
7:A:505:GOL:H32	4:D:122:CYS:HA	1.85	0.57
3:K:139:VAL:HG22	3:K:144:TYR:HB2	1.85	0.57
1:M:71:LEU:HD21	1:M:75:PHE:CE2	2.39	0.57
7:A:504:GOL:H31	12:A:695:HOH:O	2.04	0.57
4:D:102:MET:HG2	4:D:107:THR:HG23	1.86	0.57
4:L:102:MET:HG2	4:L:107:THR:HG23	1.86	0.57
2:B:104:LEU:HG	2:B:161:VAL:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:139:VAL:HG22	3:O:144:TYR:HB2	1.86	0.56
1:I:369:GLU:HG2	12:O:411:HOH:O	2.05	0.56
2:J:72:ASP:OD1	2:J:74:ASN:ND2	2.39	0.56
3:O:264:ARG:HE	3:O:264:ARG:HA	1.71	0.55
2:J:373:GLN:HG3	3:K:123:LEU:HD12	1.89	0.55
3:G:111:ARG:HG2	3:G:206:ILE:HD12	1.89	0.54
3:G:10:GLY:O	3:G:33:THR:HG21	2.07	0.54
4:H:144:ILE:HD11	4:H:184:VAL:HG21	1.89	0.54
2:N:169:GLN:HE21	7:N:403:GOL:C1	2.20	0.54
2:N:49:VAL:O	2:N:275:GLY:HA3	2.07	0.54
2:N:169:GLN:CB	7:N:403:GOL:H12	2.35	0.54
3:G:67:TYR:HE2	4:H:175:LEU:O	1.91	0.54
1:M:273:ASP:HB2	1:M:282:MET:HG2	1.90	0.53
3:O:163:SER:HB2	3:O:173:GLU:OE2	2.08	0.53
1:A:194:LYS:NZ	2:N:39:ASP:O	2.42	0.53
3:G:139:VAL:HG22	3:G:144:TYR:HB2	1.89	0.53
4:H:208:ILE:HG23	4:H:212:ILE:HD11	1.90	0.53
3:K:159:ALA:HB2	3:K:189:TYR:CD2	2.44	0.53
2:J:55:ILE:HG23	2:J:155:LEU:HD13	1.90	0.53
1:A:195:PHE:CE2	1:A:338:ILE:HD11	2.44	0.52
3:G:1:MET:HG3	3:G:2:VAL:N	2.22	0.52
4:L:122[A]:CYS:SG	4:L:202:LEU:HD22	2.48	0.52
2:F:75:GLU:HG3	2:F:97:THR:HG22	1.91	0.52
4:D:122:CYS:SG	4:D:202:LEU:HD22	2.50	0.52
3:C:139:VAL:HG22	3:C:144:TYR:HB2	1.91	0.52
1:I:283:LYS:HE2	12:I:720:HOH:O	2.10	0.52
1:A:140:GLU:CG	1:A:147:THR:HG21	2.40	0.51
1:A:195:PHE:HE2	1:A:338:ILE:HD11	1.74	0.51
1:E:76:ARG:HH22	1:E:114:MET:HE3	1.76	0.51
4:H:56:ARG:HG2	12:H:474:HOH:O	2.09	0.51
3:K:97[B]:ARG:HD2	3:K:210:SER:O	2.10	0.51
1:I:36:VAL:HG13	1:I:41:GLU:HB2	1.93	0.51
3:G:12:THR:C	3:G:33:THR:HG23	2.35	0.51
4:H:87[A]:ARG:HD3	4:H:253:PHE:CE1	2.46	0.50
3:C:35:ALA:HB1	4:D:184[B]:VAL:HG11	1.93	0.50
1:A:201[B]:ARG:NH1	1:A:334:LEU:HB3	2.27	0.50
2:B:75:GLU:HG3	2:B:97:THR:HG22	1.94	0.50
1:I:369:GLU:HG3	12:I:655:HOH:O	2.10	0.50
12:A:646:HOH:O	2:B:310:GLN:HG2	2.12	0.50
4:P:155:LYS:HE3	4:P:185:GLU:HG2	1.93	0.49
1:M:422:PRO:O	1:M:426:ARG:HG2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:34:GLY:HA2	4:L:143:ARG:HD3	1.94	0.49
1:M:71:LEU:C	1:M:71:LEU:HD23	2.37	0.49
2:B:72:ASP:OD2	4:D:231:LYS:HE3	2.12	0.49
2:J:72:ASP:OD2	4:L:231:LYS:HE3	2.13	0.49
3:C:137:LYS:NZ	3:C:171:GLU:OE1	2.46	0.49
3:C:208:VAL:HG21	3:C:234:LEU:CD1	2.42	0.48
4:D:92:MET:HA	4:D:92:MET:HE2	1.94	0.48
2:F:104:LEU:HG	2:F:161:VAL:HG21	1.95	0.48
4:H:142:LEU:HD13	4:H:184:VAL:HG23	1.94	0.48
1:A:209:ASP:OD2	7:N:403:GOL:O1	2.31	0.48
4:L:97:GLN:NE2	4:L:210:SER:O	2.43	0.48
1:M:76:ARG:HB3	1:M:76:ARG:NH1	2.29	0.48
2:J:49:VAL:O	2:J:275:GLY:HA3	2.14	0.48
1:I:80:ARG:NH1	12:I:602:HOH:O	2.40	0.48
1:I:283:LYS:HG3	1:I:310:GLY:HA2	1.95	0.47
2:J:197:TRP:CZ3	2:J:237:ARG:HG3	2.49	0.47
4:L:4:THR:HG21	4:L:255:LEU:HA	1.96	0.47
3:C:67:TYR:HE2	4:D:175:LEU:O	1.97	0.47
3:K:189:TYR:CE1	3:K:193:MET:HE3	2.49	0.47
3:C:168:VAL:HG23	4:D:168:VAL:HG23	1.96	0.47
3:C:189:TYR:CE1	3:C:193:MET:HE3	2.50	0.47
3:O:111:ARG:HG2	3:O:206:ILE:HD12	1.96	0.47
1:E:385:THR:HA	2:F:112:ASP:HB3	1.96	0.47
2:N:4:LYS:HE3	2:N:4:LYS:HB3	1.72	0.47
3:K:18:VAL:HG23	3:K:48:THR:HG22	1.96	0.47
1:A:385:THR:HA	2:B:112:ASP:HB3	1.96	0.47
2:J:159:GLU:CG	2:J:166:ILE:HD12	2.45	0.47
3:K:168:VAL:HG23	4:L:168:VAL:HG23	1.96	0.47
4:D:102:MET:HE2	4:D:102:MET:HB3	1.68	0.47
2:J:314:LYS:HG3	2:J:344:GLU:CD	2.40	0.47
1:E:72:GLN:NE2	1:E:114:MET:SD	2.83	0.46
1:I:149:ASN:HB3	12:I:641:HOH:O	2.14	0.46
1:I:394:ARG:HD2	12:I:750:HOH:O	2.16	0.46
1:I:71:LEU:HD21	1:I:75:PHE:CE2	2.51	0.46
1:I:76[B]:ARG:HA	1:I:76[B]:ARG:HD3	1.71	0.46
2:N:74[B]:ASN:ND2	4:P:200:ILE:HG21	2.31	0.46
2:F:333:ALA:HA	2:F:362:SER:O	2.16	0.46
2:J:167:THR:OG1	2:J:170:GLU:HG3	2.16	0.46
2:F:72:ASP:OD2	4:H:231:LYS:HE3	2.15	0.46
2:J:192:ARG:HD2	2:J:204:SER:HB2	1.97	0.46
1:A:201[B]:ARG:NH1	12:A:606:HOH:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ARG:HH11	1:A:76:ARG:HB3	1.80	0.46
1:E:167:GLN:HG3	1:E:168:LYS:N	2.30	0.46
3:G:119[B]:ARG:HA	3:G:119[B]:ARG:HD3	1.54	0.46
4:L:214:PHE:HB3	4:L:238:VAL:HG22	1.97	0.46
2:J:247:GLY:HA3	2:J:333:ALA:O	2.16	0.45
1:M:140:GLU:HG3	1:M:147:THR:HG21	1.96	0.45
4:P:4:THR:HG21	4:P:255:LEU:HA	1.98	0.45
3:K:122[A]:ARG:HD3	3:K:122[A]:ARG:HA	1.75	0.45
1:A:71[A]:LEU:HD12	1:A:98:TYR:OH	2.15	0.45
1:E:71:LEU:HD21	1:E:75:PHE:CE2	2.51	0.45
3:O:97[B]:ARG:HD2	3:O:210:SER:O	2.17	0.45
2:N:193:LYS:HD3	2:N:325:ALA:HA	1.98	0.45
2:B:305:PRO:HA	2:B:314:LYS:HE3	1.96	0.45
4:D:115:ASN:OD1	4:D:115:ASN:N	2.49	0.45
3:K:111:ARG:HD3	3:K:207:ASN:O	2.16	0.45
4:L:115:ASN:HB2	4:L:117:GLU:H	1.81	0.45
1:A:201[B]:ARG:HD2	1:A:334:LEU:O	2.15	0.45
3:C:232:LEU:HD22	3:C:234:LEU:HD12	1.99	0.45
1:I:381:LYS:HA	2:J:83:TYR:CD2	2.52	0.45
4:H:102:MET:HG2	4:H:107:THR:HG23	1.98	0.45
2:F:386:MET:O	2:F:388:ASP:N	2.50	0.45
2:F:382:VAL:O	2:F:385:ILE:HG13	2.17	0.45
1:I:385:THR:HA	2:J:112:ASP:HB3	1.98	0.45
3:K:131:THR:HG21	3:K:195:LEU:HD13	1.99	0.45
12:J:533:HOH:O	4:L:204:ARG:HD2	2.17	0.45
3:K:81:ASP:OD1	3:K:81:ASP:N	2.50	0.45
2:J:155:LEU:HD11	2:J:166:ILE:HD13	1.98	0.44
1:A:426:ARG:HG2	12:A:644:HOH:O	2.17	0.44
4:D:159:PRO:HB3	4:D:189:TRP:HD1	1.83	0.44
1:E:182:GLU:OE2	2:F:141:LYS:HG2	2.18	0.44
1:M:381:LYS:HA	2:N:83:TYR:CD2	2.53	0.44
2:N:8:GLY:O	2:N:12:LYS:HE2	2.17	0.44
2:B:42:ARG:HB2	2:B:61:LEU:HD22	2.00	0.44
1:A:241:ALA:O	1:A:245:ARG:HB2	2.18	0.44
3:K:125:ASP:OD2	3:K:198[B]:ARG:NH2	2.51	0.44
4:H:122:CYS:SG	4:H:202:LEU:HD22	2.58	0.44
1:M:36:VAL:HG13	1:M:41:GLU:HB2	2.00	0.44
2:F:49:VAL:O	2:F:275:GLY:HA3	2.18	0.44
2:B:354:GLU:OE1	12:B:501:HOH:O	2.21	0.44
1:I:71:LEU:C	1:I:71:LEU:HD23	2.42	0.44
4:H:1:MET:HG2	4:H:3:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:78:VAL:HA	12:I:734:HOH:O	2.17	0.43
1:E:381:LYS:HA	2:F:83:TYR:CD2	2.53	0.43
4:P:122:CYS:SG	4:P:202:LEU:HD22	2.57	0.43
1:E:167:GLN:NE2	12:E:609:HOH:O	2.51	0.43
2:B:247:GLY:HA3	2:B:333:ALA:O	2.18	0.43
2:B:49:VAL:O	2:B:275:GLY:HA3	2.18	0.43
2:B:201:ALA:HB2	2:B:267:VAL:HB	2.00	0.43
3:K:111:ARG:NH1	3:K:207:ASN:O	2.48	0.43
2:B:254:PRO:HG3	2:B:366:GLU:O	2.18	0.43
1:I:426:ARG:HG3	1:I:426:ARG:HH11	1.83	0.43
2:N:169:GLN:HE21	7:N:403:GOL:H11	1.84	0.43
2:B:36:TRP:CE2	2:B:62:LEU:HB2	2.54	0.42
3:K:107:MET:HG3	3:K:124:ASN:HB3	2.01	0.42
2:N:247:GLY:HA3	2:N:333:ALA:O	2.20	0.42
4:P:17:VAL:HG13	4:P:25:ILE:HG23	2.02	0.42
1:A:238:MET:HE3	1:A:238:MET:HB3	1.79	0.42
12:A:609:HOH:O	2:B:310:GLN:NE2	2.53	0.42
3:C:193:MET:HE1	3:C:227:ALA:HB2	2.00	0.42
2:J:36:TRP:CE2	2:J:62:LEU:HB2	2.55	0.42
4:D:99:VAL:HB	4:D:110:ILE:HB	2.01	0.42
2:N:281:GLU:OE1	2:N:300:HIS:ND1	2.50	0.42
3:O:133:MET:O	3:O:137:LYS:HG3	2.20	0.42
3:O:200:VAL:HG11	3:O:231:GLU:HG3	2.01	0.42
1:A:136:GLY:HA2	1:A:139:TRP:CE3	2.55	0.42
1:M:421:ALA:HB3	1:M:422:PRO:HD3	2.02	0.42
1:A:232:THR:HA	1:A:299:TYR:OH	2.20	0.41
1:A:436:SER:O	1:A:440:GLN:N	2.50	0.41
1:E:114:MET:HE2	1:E:114:MET:HB3	1.93	0.41
1:E:274:LYS:HB2	1:E:274:LYS:HE3	1.81	0.41
3:O:119:ARG:HA	3:O:119:ARG:HD3	1.74	0.41
4:D:215:THR:HG22	4:D:245:MET:HG3	2.02	0.41
2:F:338:CYS:HA	5:F:401:SF4:S1	2.61	0.41
3:C:163:SER:CB	3:C:173:GLU:OE2	2.69	0.41
1:E:77:ASN:ND2	12:E:610:HOH:O	2.51	0.41
1:M:76:ARG:HG3	1:M:114[B]:MET:HE2	2.02	0.41
1:M:141:ARG:NH2	12:M:605:HOH:O	2.45	0.41
3:C:11:SER:HA	3:C:67:TYR:CE1	2.56	0.41
3:G:189:TYR:CE1	3:G:193:MET:HE3	2.55	0.41
3:G:193:MET:HE1	3:G:227:ALA:CB	2.51	0.41
3:K:193:MET:HE1	3:K:227:ALA:HB2	2.02	0.41
3:O:67:TYR:HE2	4:P:175:LEU:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:168:VAL:HG23	4:P:168:VAL:HG23	2.02	0.41
4:L:142:LEU:CD2	4:L:178:LEU:HD11	2.50	0.41
1:A:379:PRO:HD2	1:A:408:ILE:O	2.20	0.41
1:E:164:ARG:NE	1:E:343:GLU:OE1	2.53	0.41
3:O:81:ASP:OD1	3:O:81:ASP:N	2.51	0.41
1:I:421:ALA:HB3	1:I:422:PRO:HD3	2.02	0.41
4:P:1:MET:SD	4:P:21:GLU:HG2	2.61	0.41
2:B:139:ASN:OD1	2:B:310:GLN:HG3	2.21	0.41
3:G:163:SER:N	3:G:173:GLU:OE2	2.54	0.41
1:I:232:THR:HA	1:I:299:TYR:OH	2.20	0.41
2:J:169:GLN:CD	2:J:169:GLN:H	2.29	0.41
2:N:254:PRO:HG3	2:N:366:GLU:O	2.20	0.41
4:P:92:MET:HA	4:P:92:MET:HE2	2.02	0.41
3:C:91:PHE:CD1	3:C:250:LEU:HD21	2.56	0.40
1:I:300:ARG:HA	1:I:300:ARG:HD3	1.92	0.40
2:J:101:GLU:HG3	12:N:505:HOH:O	2.21	0.40
2:J:104:LEU:HG	2:J:161:VAL:HG21	2.03	0.40
3:K:137:LYS:NZ	4:L:171:GLU:OE2	2.53	0.40
2:F:364:PHE:HA	2:F:368:GLN:OE1	2.21	0.40
2:F:388:ASP:HA	3:G:117:LYS:NZ	2.36	0.40
4:H:65:THR:C	4:H:69:ARG:HB3	2.47	0.40
1:A:112:HIS:CE1	1:A:114:MET:HG3	2.57	0.40
3:G:193:MET:HE1	3:G:227:ALA:HB2	2.03	0.40
3:K:1:MET:SD	3:K:20:ASP:HB2	2.62	0.40
3:O:47:GLU:O	3:O:51:GLN:HG3	2.21	0.40
3:O:200:VAL:HG12	3:O:204:LYS:HE2	2.03	0.40
2:B:8:GLY:O	2:B:12:LYS:HE2	2.20	0.40
1:E:102:GLY:O	1:E:106:GLN:HG3	2.20	0.40
12:F:566:HOH:O	2:N:356:LYS:HE3	2.22	0.40
2:J:196:PRO:HD2	2:J:197:TRP:CZ3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/445 (99%)	430 (98%)	8 (2%)	3 (1%)	18	10
1	E	437/445 (98%)	427 (98%)	7 (2%)	3 (1%)	18	10
1	I	437/445 (98%)	426 (98%)	9 (2%)	2 (0%)	24	16
1	M	438/445 (98%)	425 (97%)	10 (2%)	3 (1%)	18	10
2	B	389/388 (100%)	381 (98%)	8 (2%)	0	100	100
2	F	387/388 (100%)	379 (98%)	7 (2%)	1 (0%)	36	29
2	J	386/388 (100%)	376 (97%)	9 (2%)	1 (0%)	36	29
2	N	389/388 (100%)	381 (98%)	8 (2%)	0	100	100
3	C	265/273 (97%)	261 (98%)	3 (1%)	1 (0%)	30	22
3	G	265/273 (97%)	261 (98%)	4 (2%)	0	100	100
3	K	268/273 (98%)	262 (98%)	5 (2%)	1 (0%)	30	22
3	O	266/273 (97%)	261 (98%)	5 (2%)	0	100	100
4	D	263/269 (98%)	261 (99%)	2 (1%)	0	100	100
4	H	261/269 (97%)	260 (100%)	1 (0%)	0	100	100
4	L	262/269 (97%)	261 (100%)	1 (0%)	0	100	100
4	P	260/269 (97%)	259 (100%)	1 (0%)	0	100	100
All	All	5414/5500 (98%)	5311 (98%)	88 (2%)	15 (0%)	36	29

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	387	PHE
3	C	207	ASN
3	K	207	ASN
1	M	410	SER
1	A	410	SER
1	E	410	SER
1	I	410	SER
2	J	302	SER
1	A	413	VAL
1	E	413	VAL
1	I	413	VAL
1	M	52	VAL
1	M	413	VAL
1	A	52	VAL

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Mol	Chain	Res	Type
1	E	52	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	372/371 (100%)	366 (98%)	6 (2%)	55	54
1	E	369/371 (100%)	363 (98%)	6 (2%)	55	54
1	I	368/371 (99%)	362 (98%)	6 (2%)	55	54
1	M	369/371 (100%)	363 (98%)	6 (2%)	55	54
2	B	339/336 (101%)	336 (99%)	3 (1%)	70	73
2	F	337/336 (100%)	334 (99%)	3 (1%)	70	73
2	J	336/336 (100%)	334 (99%)	2 (1%)	78	81
2	N	339/336 (101%)	337 (99%)	2 (1%)	78	81
3	C	214/215 (100%)	210 (98%)	4 (2%)	50	47
3	G	214/215 (100%)	209 (98%)	5 (2%)	44	40
3	K	217/215 (101%)	212 (98%)	5 (2%)	44	40
3	O	214/215 (100%)	205 (96%)	9 (4%)	26	19
4	D	201/203 (99%)	198 (98%)	3 (2%)	57	56
4	H	199/203 (98%)	195 (98%)	4 (2%)	48	46
4	L	200/203 (98%)	194 (97%)	6 (3%)	36	30
4	P	198/203 (98%)	193 (98%)	5 (2%)	42	37
All	All	4486/4500 (100%)	4411 (98%)	75 (2%)	53	52

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	8	THR
1	A	76	ARG

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Mol	Chain	Res	Type
1	A	114	MET
1	A	151	ASP
1	A	238	MET
2	B	314	LYS
2	B	362	SER
2	B	376	ILE
3	C	81	ASP
3	C	119	ARG
3	C	139	VAL
3	C	171	GLU
4	D	56	ARG
4	D	115	ASN
4	D	239	SER
1	E	57	ARG
1	E	167	GLN
1	E	218	LEU
1	E	412	LEU
1	E	437	ARG
1	E	439	GLN
2	F	15	GLU
2	F	152	ARG
2	F	388	ASP
3	G	1	MET
3	G	56	LYS
3	G	139	VAL
3	G	262	LYS
3	G	264	ARG
4	H	56	ARG
4	H	115	ASN
4	H	230	GLU
4	H	239	SER
1	I	8	THR
1	I	10	GLU
1	I	57	ARG
1	I	222	ARG
1	I	412	LEU
1	I	440	GLN
2	J	169	GLN
2	J	376	ILE
3	K	1	MET
3	K	81	ASP
3	K	107	MET

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Mol	Chain	Res	Type
3	K	139	VAL
3	K	262	LYS
4	L	39	GLN
4	L	51	SER
4	L	100	ILE
4	L	106	ASP
4	L	140	ASP
4	L	212	ILE
1	M	6	GLN
1	M	8	THR
1	M	151	ASP
1	M	335	ASN
1	M	412	LEU
1	M	434	LEU
2	N	15	GLU
2	N	376	ILE
3	O	1	MET
3	O	12	THR
3	O	53	LYS
3	O	81	ASP
3	O	139	VAL
3	O	145[A]	ASP
3	O	145[B]	ASP
3	O	233	ASN
3	O	264	ARG
4	P	2	LYS
4	P	100	ILE
4	P	185	GLU
4	P	235	LYS
4	P	239	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	235	ASN
2	B	300	HIS
3	C	46	ASN
3	C	105	GLN
3	C	180	ASN
3	C	233	ASN
1	E	149	ASN
1	E	167	GLN

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Mol	Chain	Res	Type
1	E	202	GLN
2	F	234	GLN
2	F	300	HIS
3	G	24	ASN
4	H	39	GLN
1	I	72	GLN
1	I	149	ASN
1	I	235	ASN
1	I	345	GLN
2	J	194	ASN
2	J	259	GLN
2	J	300	HIS
2	J	373	GLN
3	K	24	ASN
2	N	16	GLN
3	O	24	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 60 ligands modelled in this entry, 30 are monoatomic - leaving 30 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SF4	E	501	1	0,12,12	-	-	-		
7	GOL	N	403	-	5,5,5	1.17	0	5,5,5	0.53	0
10	ATP	O	301	9	32,33,33	0.95	2 (6%)	48,52,52	0.51	0
5	SF4	K	303	3,4	0,12,12	-	-	-		
5	SF4	F	401	2	0,12,12	-	-	-		
5	SF4	M	501	12,1	0,12,12	-	-	-		
7	GOL	I	503	-	5,5,5	1.08	0	5,5,5	0.93	0
7	GOL	A	504	-	5,5,5	0.74	0	5,5,5	0.68	0
5	SF4	B	401	2	0,12,12	-	-	-		
5	SF4	J	401	2	0,12,12	-	-	-		
7	GOL	M	504	-	5,5,5	1.22	0	5,5,5	0.92	0
10	ATP	C	301	9	32,33,33	0.65	1 (3%)	48,52,52	0.52	0
11	ADP	D	301	9	28,29,29	1.50	5 (17%)	43,45,45	1.71	10 (23%)
5	SF4	I	501	1	0,12,12	-	-	-		
10	ATP	K	301	9	32,33,33	0.84	2 (6%)	48,52,52	0.43	0
7	GOL	I	504	-	5,5,5	0.97	0	5,5,5	0.80	0
5	SF4	O	303	3,4	0,12,12	-	-	-		
7	GOL	A	505	-	5,5,5	1.35	1 (20%)	5,5,5	0.79	0
11	ADP	P	301	9	28,29,29	1.42	6 (21%)	43,45,45	1.79	10 (23%)
5	SF4	G	303	3,4	0,12,12	-	-	-		
7	GOL	E	505	-	5,5,5	0.78	0	5,5,5	0.89	0
10	ATP	G	301	9	32,33,33	0.58	1 (3%)	48,52,52	0.48	0
7	GOL	A	503	-	5,5,5	1.51	1 (20%)	5,5,5	0.89	0
5	SF4	A	501	12,1	0,12,12	-	-	-		
5	SF4	N	401	2	0,12,12	-	-	-		
11	ADP	L	301	9	28,29,29	1.42	5 (17%)	43,45,45	1.83	10 (23%)
11	ADP	H	301	9	28,29,29	1.57	6 (21%)	43,45,45	1.73	10 (23%)
5	SF4	C	303	3,4	0,12,12	-	-	-		
7	GOL	E	504	-	5,5,5	1.18	1 (20%)	5,5,5	0.99	0
7	GOL	M	505	-	5,5,5	0.77	0	5,5,5	0.96	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SF4	E	501	1	-	-	0/6/5/5
7	GOL	N	403	-	-	2/4/4/4	-
10	ATP	O	301	9	-	3/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SF4	K	303	3,4	-	-	0/6/5/5
5	SF4	F	401	2	-	-	0/6/5/5
7	GOL	I	503	-	-	0/4/4/4	-
5	SF4	M	501	12,1	-	-	0/6/5/5
7	GOL	A	504	-	-	2/4/4/4	-
5	SF4	B	401	2	-	-	0/6/5/5
10	ATP	C	301	9	-	4/22/38/38	0/3/3/3
7	GOL	M	504	-	-	0/4/4/4	-
5	SF4	J	401	2	-	-	0/6/5/5
11	ADP	D	301	9	-	0/16/32/32	0/3/3/3
10	ATP	K	301	9	-	3/22/38/38	0/3/3/3
5	SF4	I	501	1	-	-	0/6/5/5
7	GOL	I	504	-	-	2/4/4/4	-
5	SF4	O	303	3,4	-	-	0/6/5/5
7	GOL	A	505	-	-	2/4/4/4	-
11	ADP	P	301	9	-	0/16/32/32	0/3/3/3
5	SF4	G	303	3,4	-	-	0/6/5/5
7	GOL	E	505	-	-	0/4/4/4	-
10	ATP	G	301	9	-	3/22/38/38	0/3/3/3
7	GOL	A	503	-	-	0/4/4/4	-
5	SF4	A	501	12,1	-	-	0/6/5/5
11	ADP	L	301	9	-	0/16/32/32	0/3/3/3
5	SF4	N	401	2	-	-	0/6/5/5
11	ADP	H	301	9	-	0/16/32/32	0/3/3/3
5	SF4	C	303	3,4	-	-	0/6/5/5
7	GOL	E	504	-	-	0/4/4/4	-
7	GOL	M	505	-	-	0/4/4/4	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	301	ADP	C5-C4	4.56	1.47	1.39
11	P	301	ADP	C5-C4	4.54	1.47	1.39
11	H	301	ADP	C5-C4	4.44	1.47	1.39
11	L	301	ADP	C5-C4	4.38	1.46	1.39
10	O	301	ATP	PA-O3A	-3.94	1.55	1.59
10	K	301	ATP	PA-O3A	-3.83	1.55	1.59
11	H	301	ADP	PA-O3A	3.51	1.63	1.59
11	D	301	ADP	PA-O3A	3.30	1.63	1.59
10	O	301	ATP	PB-O3B	-3.26	1.56	1.59
10	C	301	ATP	PA-O3A	-3.17	1.56	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	505	GOL	O2-C2	-2.80	1.35	1.43
11	D	301	ADP	C5-C6	2.74	1.48	1.41
11	H	301	ADP	C5-C6	2.72	1.48	1.41
7	A	503	GOL	C1-C2	2.62	1.61	1.51
11	P	301	ADP	C5-C6	2.58	1.48	1.41
11	H	301	ADP	C8-N7	2.55	1.36	1.31
11	L	301	ADP	PA-O3A	2.53	1.62	1.59
11	P	301	ADP	C8-N7	2.48	1.36	1.31
11	L	301	ADP	C5-C6	2.46	1.47	1.41
11	D	301	ADP	C8-N7	2.45	1.36	1.31
10	G	301	ATP	PB-O3B	-2.45	1.56	1.59
11	H	301	ADP	C4-N9	-2.41	1.32	1.37
11	L	301	ADP	C5-N7	-2.38	1.34	1.39
11	P	301	ADP	PA-O3A	2.30	1.62	1.59
11	P	301	ADP	C5-N7	-2.16	1.35	1.39
10	K	301	ATP	PB-O3B	-2.15	1.57	1.59
7	E	504	GOL	C3-C2	2.14	1.59	1.51
11	P	301	ADP	C4-N9	-2.12	1.33	1.37
11	H	301	ADP	C5-N7	-2.11	1.35	1.39
11	L	301	ADP	C8-N7	2.04	1.35	1.31
11	D	301	ADP	C4-N9	-2.01	1.33	1.37

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	301	ADP	C5-C4-N3	-5.27	119.46	126.72
11	P	301	ADP	C5-C4-N3	-4.96	119.88	126.72
11	D	301	ADP	C5-C4-N3	-4.94	119.91	126.72
11	L	301	ADP	N3-C4-N9	4.62	135.03	127.17
11	H	301	ADP	C5-C4-N3	-4.59	120.39	126.72
11	P	301	ADP	N3-C2-N1	-3.95	122.60	128.58
11	D	301	ADP	N3-C4-N9	3.91	133.82	127.17
11	H	301	ADP	N3-C4-N9	3.82	133.66	127.17
11	P	301	ADP	N3-C4-N9	3.79	133.62	127.17
11	P	301	ADP	C4-C5-N7	-3.71	106.34	110.58
11	P	301	ADP	C2-N3-C4	3.60	120.63	111.83
11	H	301	ADP	C4-N9-C8	3.60	109.51	105.74
11	H	301	ADP	N3-C2-N1	-3.56	123.20	128.58
11	L	301	ADP	C4-N9-C8	3.55	109.47	105.74
11	D	301	ADP	C4-C5-N7	-3.46	106.63	110.58
11	L	301	ADP	C2-N3-C4	3.34	120.00	111.83
11	D	301	ADP	N3-C2-N1	-3.22	123.71	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	301	ADP	C2-N3-C4	3.21	119.68	111.83
11	L	301	ADP	N3-C2-N1	-3.20	123.74	128.58
11	D	301	ADP	C4-N9-C8	3.18	109.07	105.74
11	H	301	ADP	C2-N3-C4	3.18	119.59	111.83
11	L	301	ADP	C4-C5-N7	-3.16	106.97	110.58
11	P	301	ADP	C4-N9-C8	3.08	108.97	105.74
11	H	301	ADP	C4-C5-N7	-3.03	107.12	110.58
11	L	301	ADP	C5-N7-C8	2.79	107.83	103.45
11	P	301	ADP	C5-N7-C8	2.78	107.81	103.45
11	P	301	ADP	C2-N1-C6	2.70	123.17	118.73
11	H	301	ADP	N9-C8-N7	-2.62	110.22	113.94
11	L	301	ADP	N9-C8-N7	-2.62	110.22	113.94
11	H	301	ADP	C2-N1-C6	2.59	122.98	118.73
11	P	301	ADP	C6-C5-N7	2.56	137.02	132.09
11	P	301	ADP	N9-C8-N7	-2.51	110.37	113.94
11	D	301	ADP	C5-N7-C8	2.50	107.39	103.45
11	H	301	ADP	C5-N7-C8	2.39	107.20	103.45
11	D	301	ADP	N9-C8-N7	-2.32	110.64	113.94
11	D	301	ADP	C2-N1-C6	2.32	122.54	118.73
11	L	301	ADP	O2A-PA-O1A	2.24	122.84	112.44
11	D	301	ADP	C6-C5-N7	2.18	136.29	132.09
11	L	301	ADP	O2'-C2'-C1'	-2.12	102.79	110.10
11	H	301	ADP	C6-C5-N7	2.07	136.08	132.09

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	504	GOL	O1-C1-C2-C3
7	A	505	GOL	C1-C2-C3-O3
7	A	505	GOL	O2-C2-C3-O3
7	I	504	GOL	O1-C1-C2-C3
7	N	403	GOL	C1-C2-C3-O3
7	A	504	GOL	O1-C1-C2-O2
7	N	403	GOL	O2-C2-C3-O3
10	G	301	ATP	PB-O3B-PG-O1G
10	C	301	ATP	PB-O3B-PG-O2G
10	G	301	ATP	PB-O3B-PG-O2G
10	G	301	ATP	PG-O3B-PB-O1B
10	C	301	ATP	PB-O3B-PG-O1G
10	K	301	ATP	PB-O3B-PG-O1G
10	O	301	ATP	PB-O3B-PG-O1G

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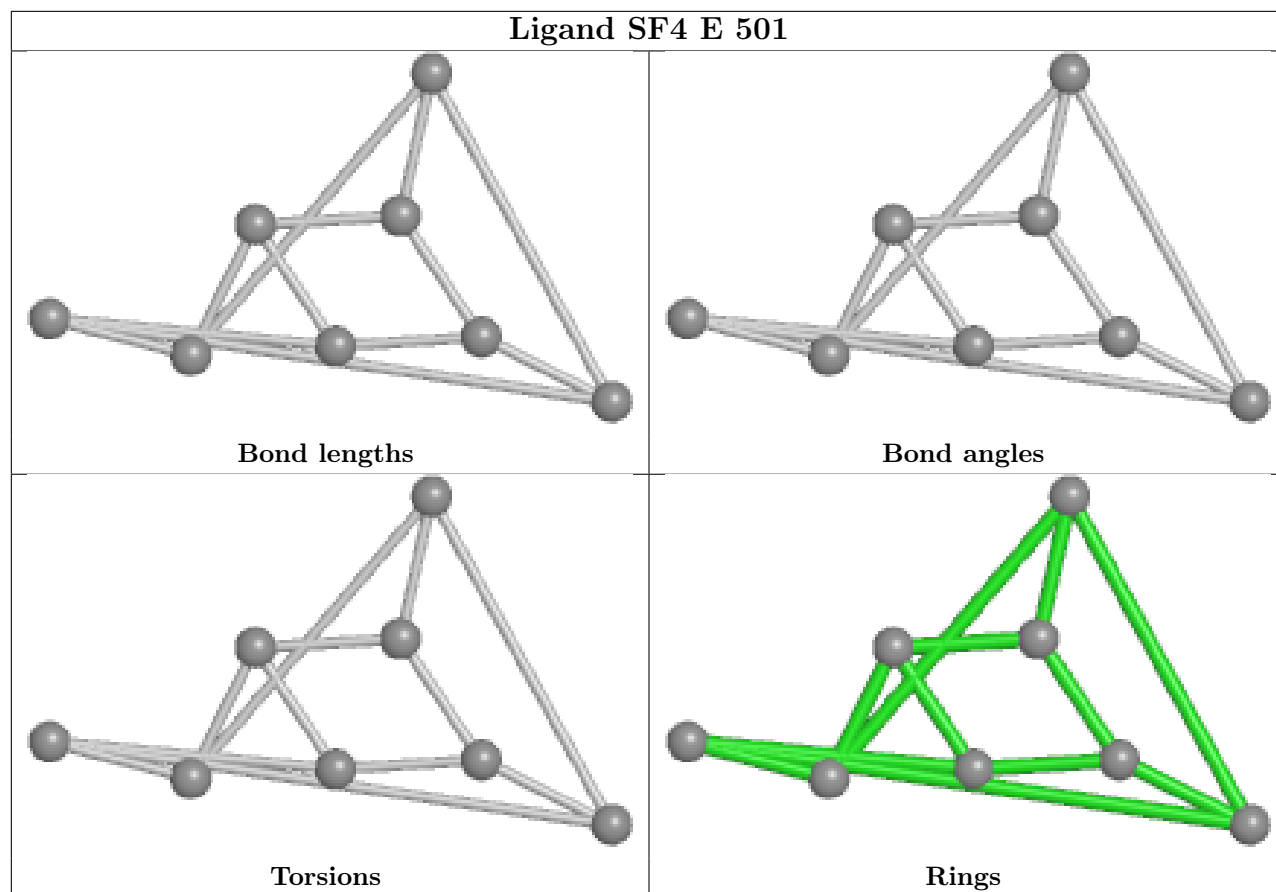
Mol	Chain	Res	Type	Atoms
7	I	504	GOL	O1-C1-C2-O2
10	K	301	ATP	PG-O3B-PB-O1B
10	C	301	ATP	PG-O3B-PB-O1B
10	O	301	ATP	PG-O3B-PB-O1B
10	C	301	ATP	PG-O3B-PB-O2B
10	K	301	ATP	PG-O3B-PB-O2B
10	O	301	ATP	PG-O3B-PB-O2B

There are no ring outliers.

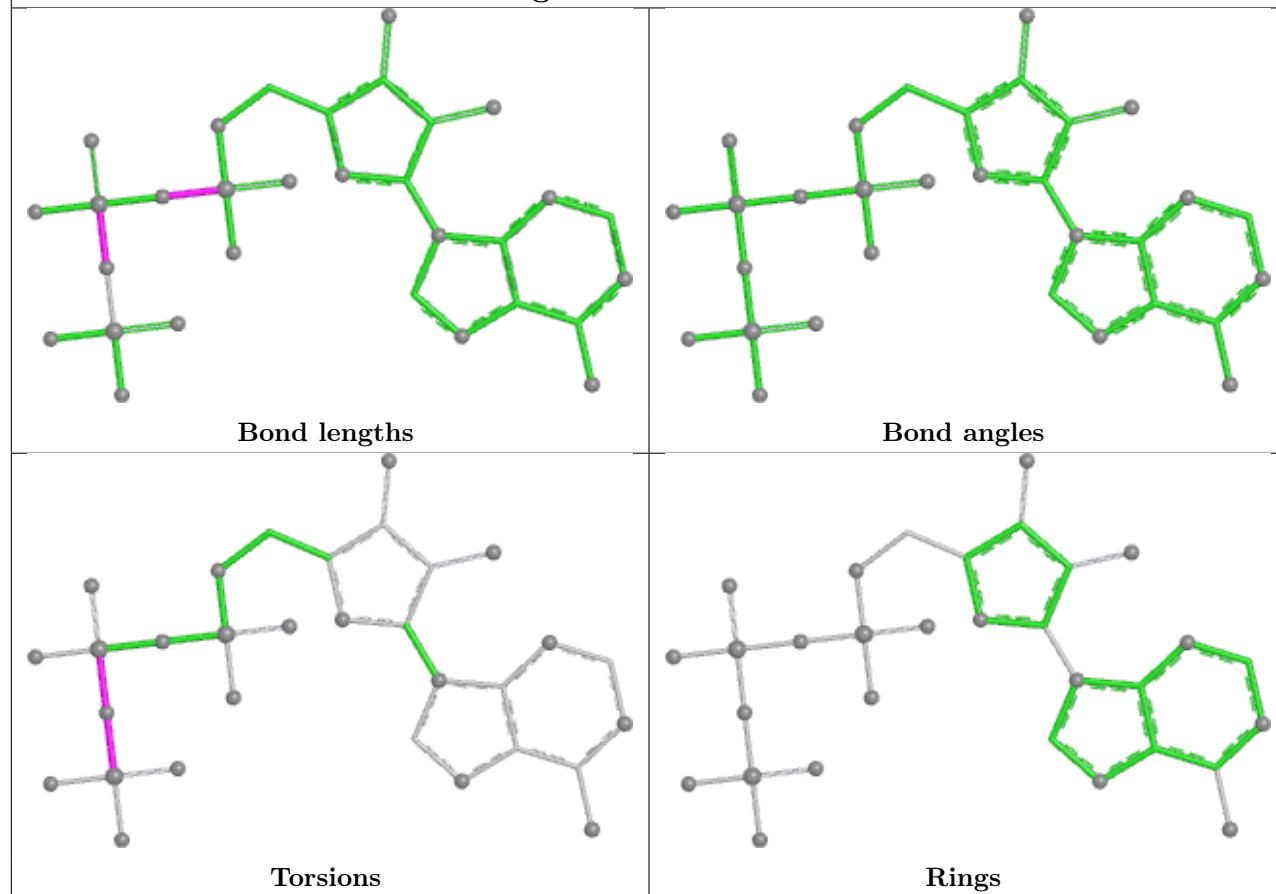
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	N	403	GOL	5	0
5	F	401	SF4	1	0
7	A	504	GOL	1	0
7	A	505	GOL	1	0

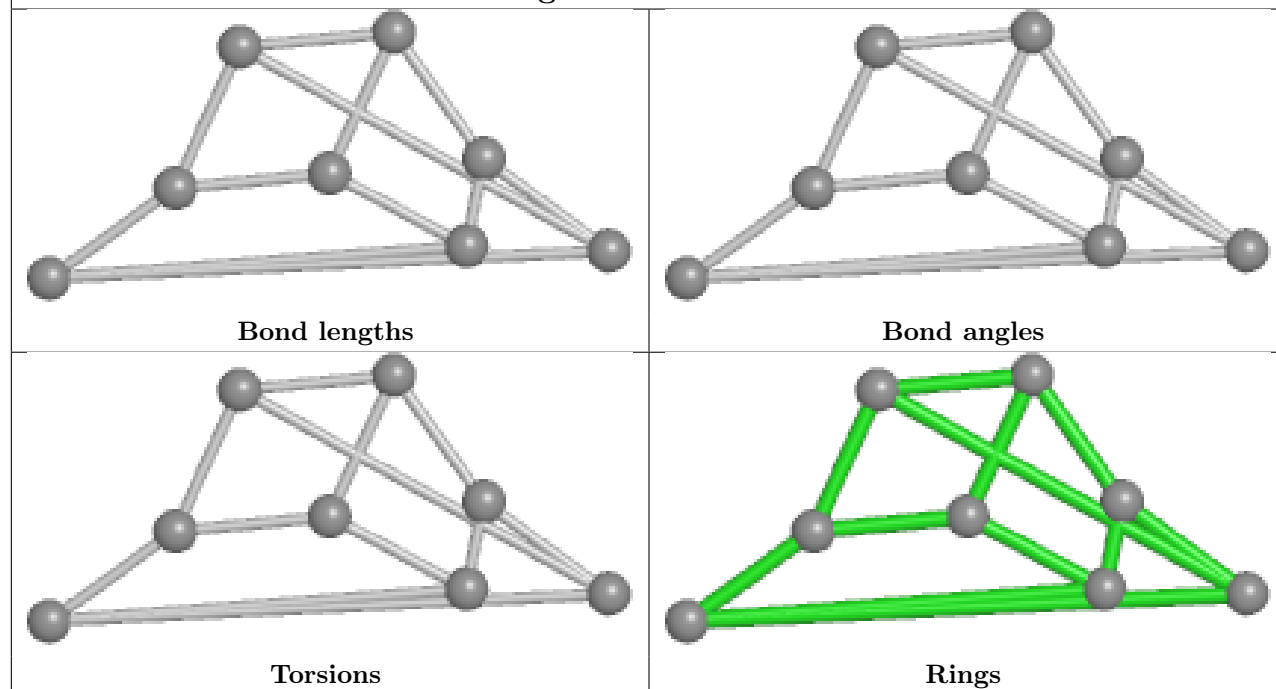
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

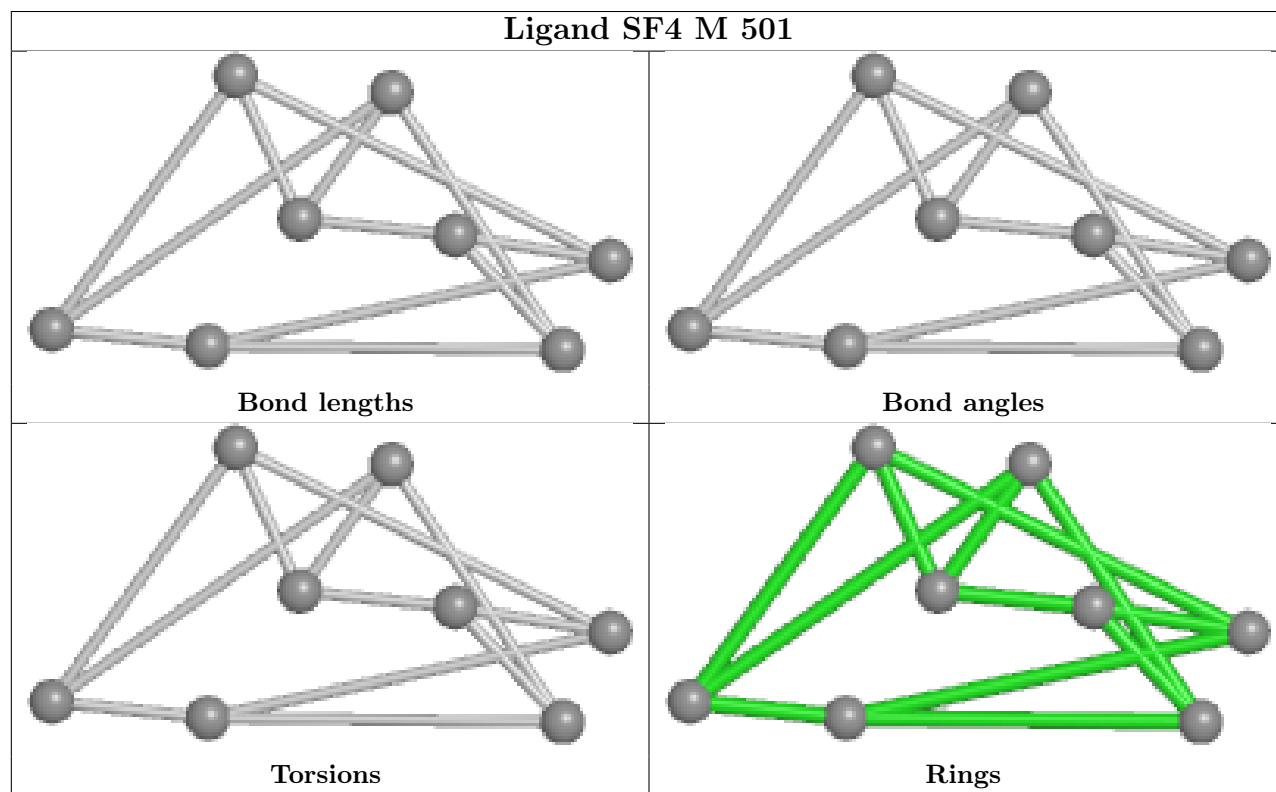
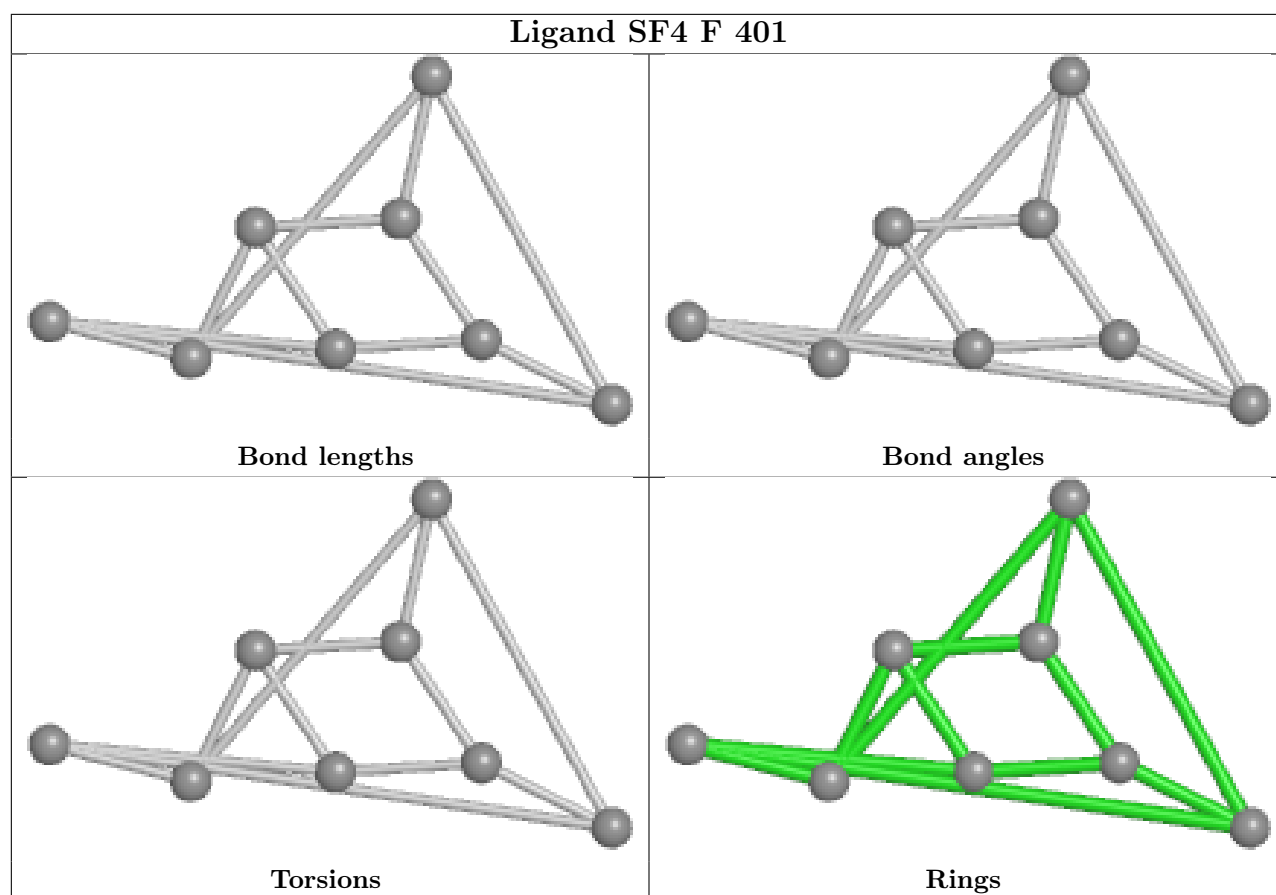


Ligand ATP O 301

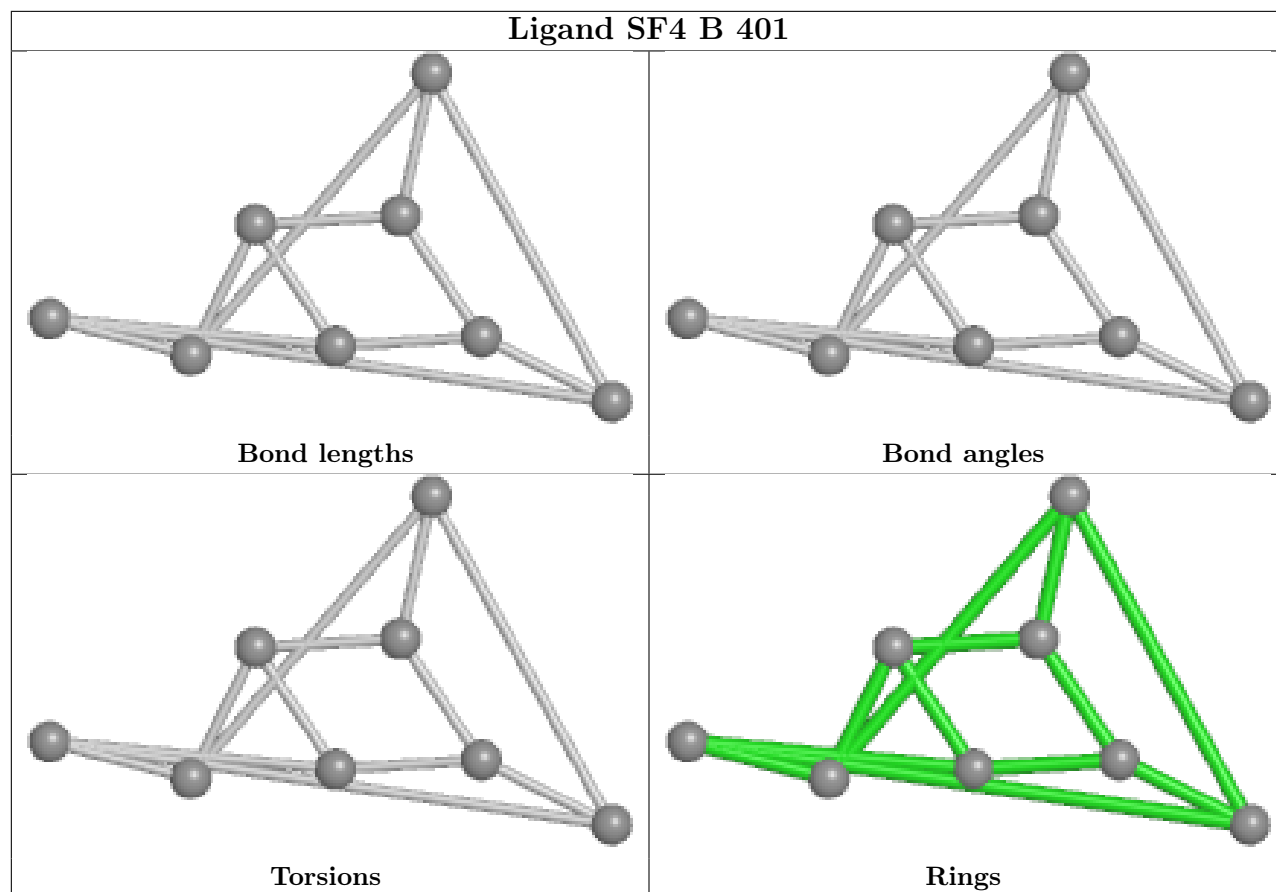


Ligand SF4 K 303

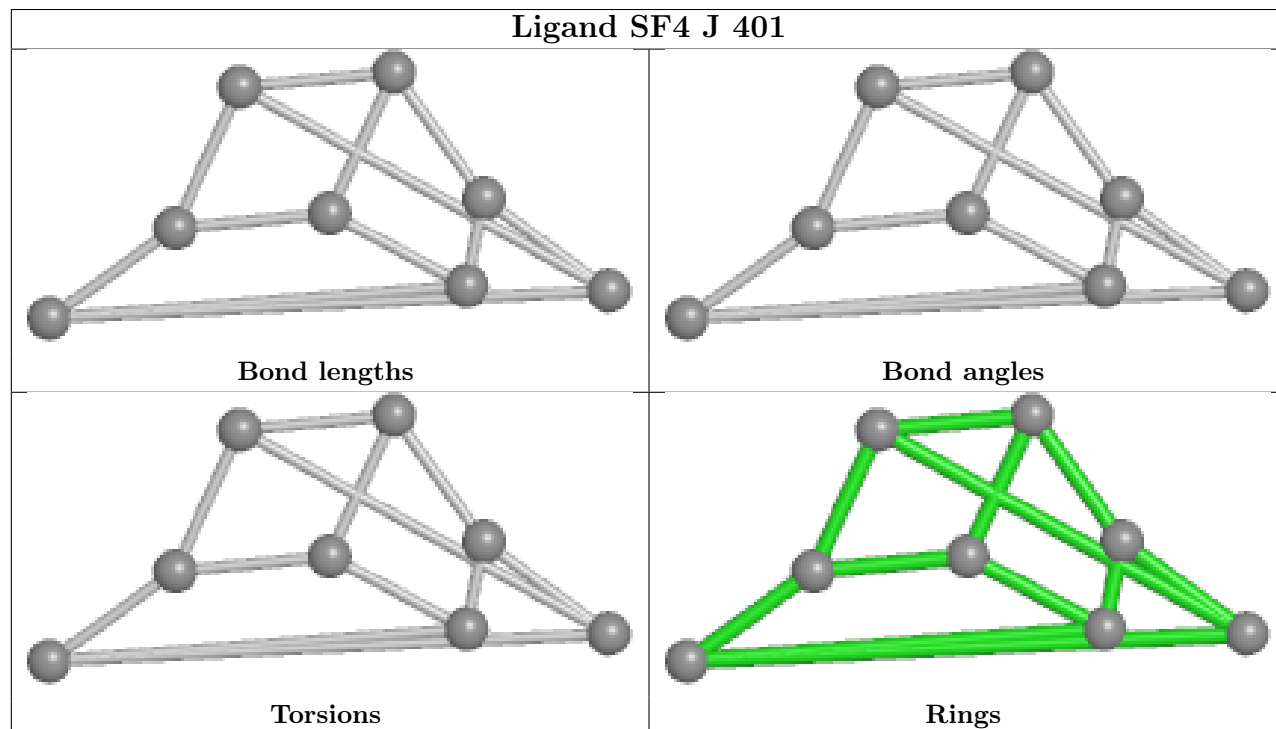




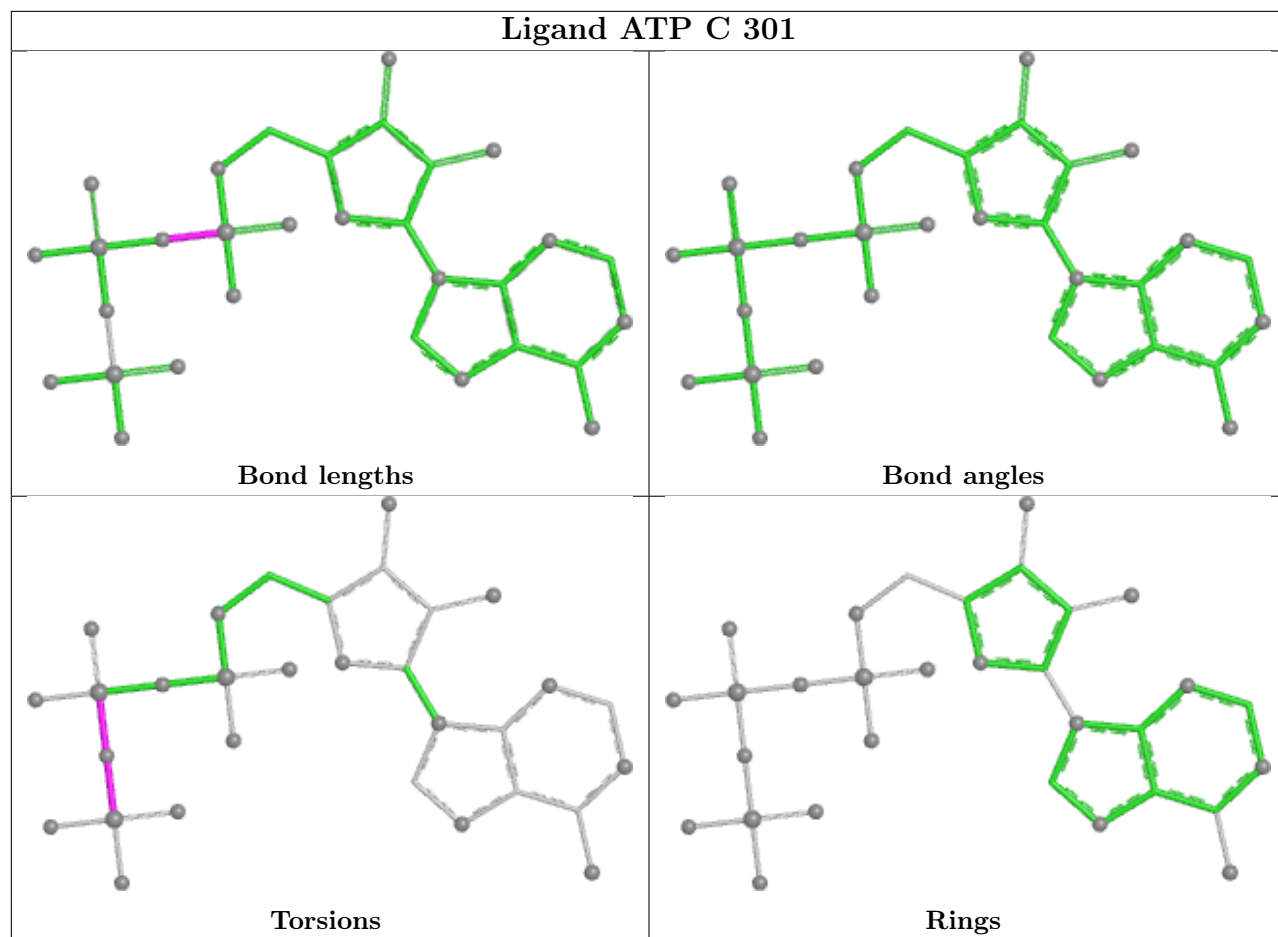
Ligand SF4 B 401



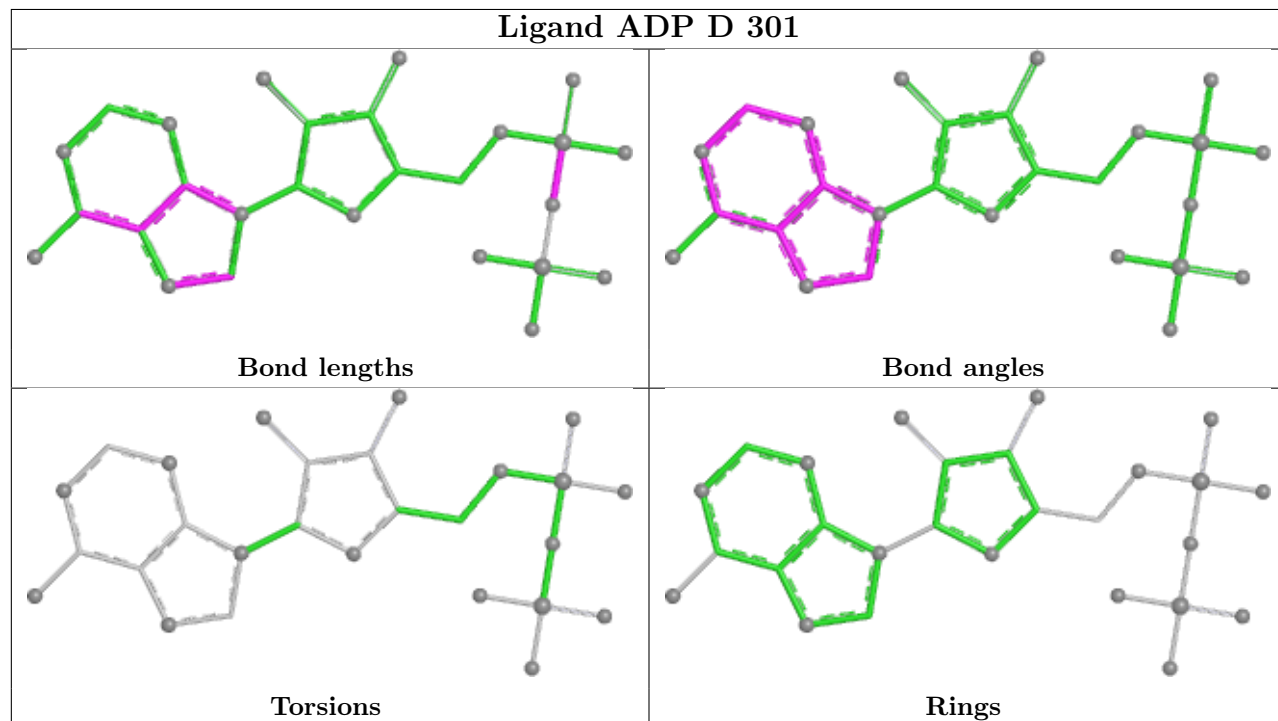
Ligand SF4 J 401



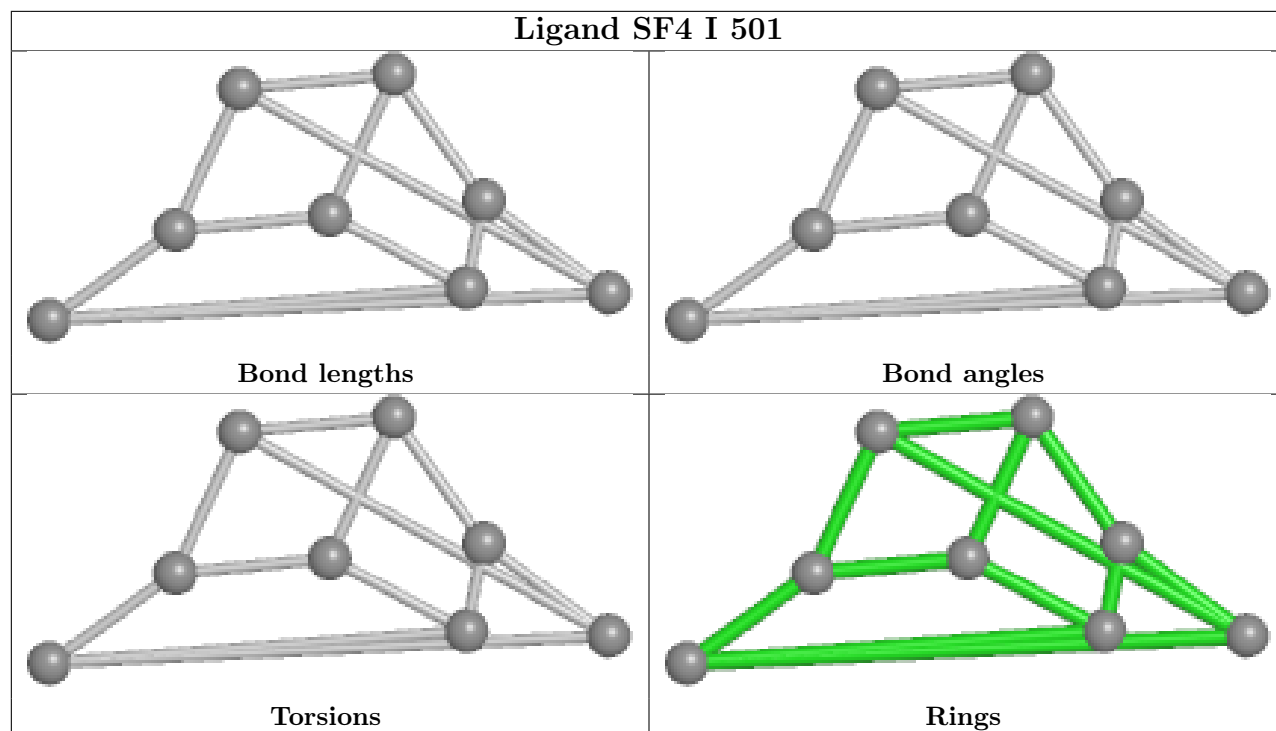
Ligand ATP C 301



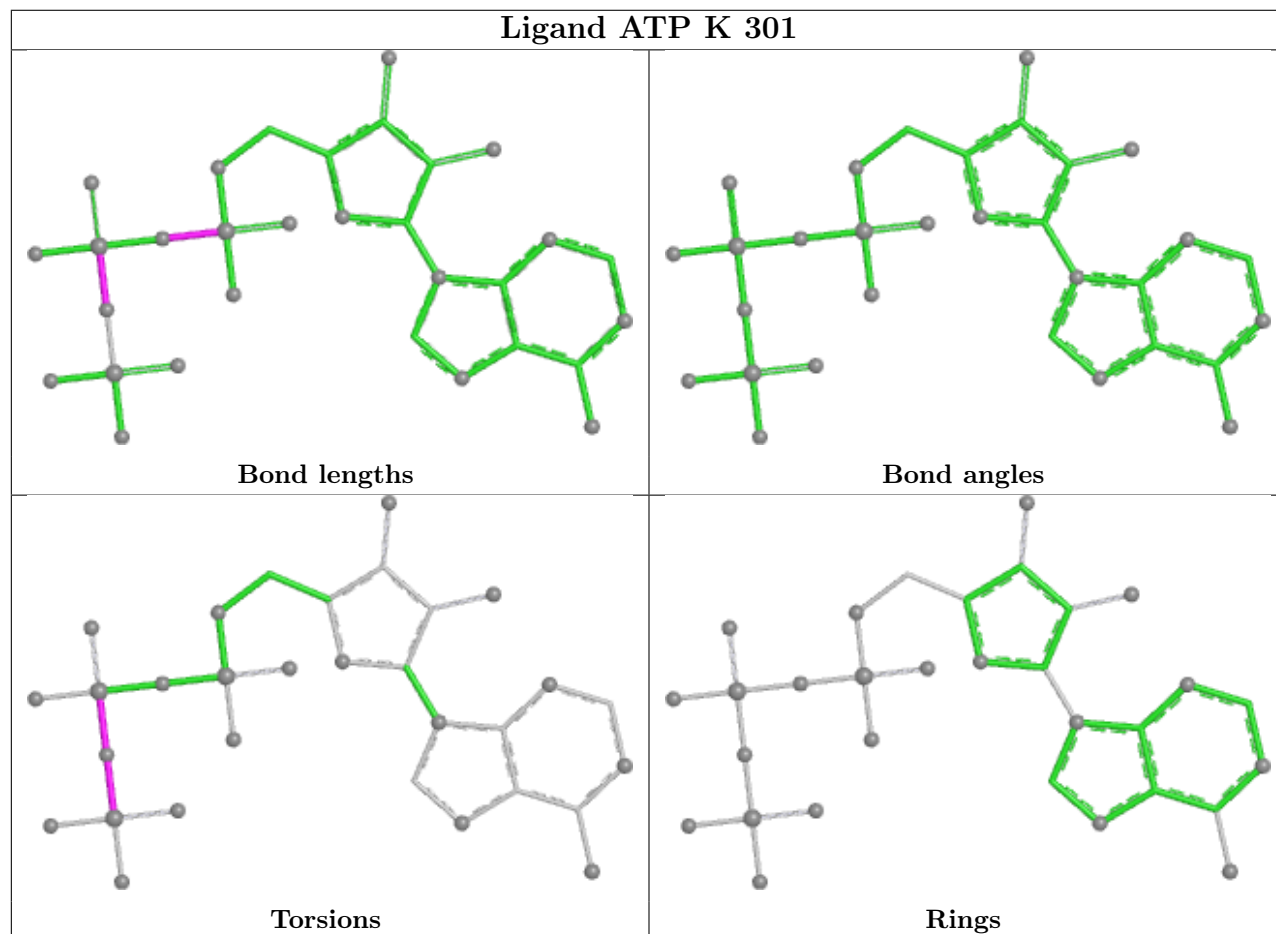
Ligand ADP D 301



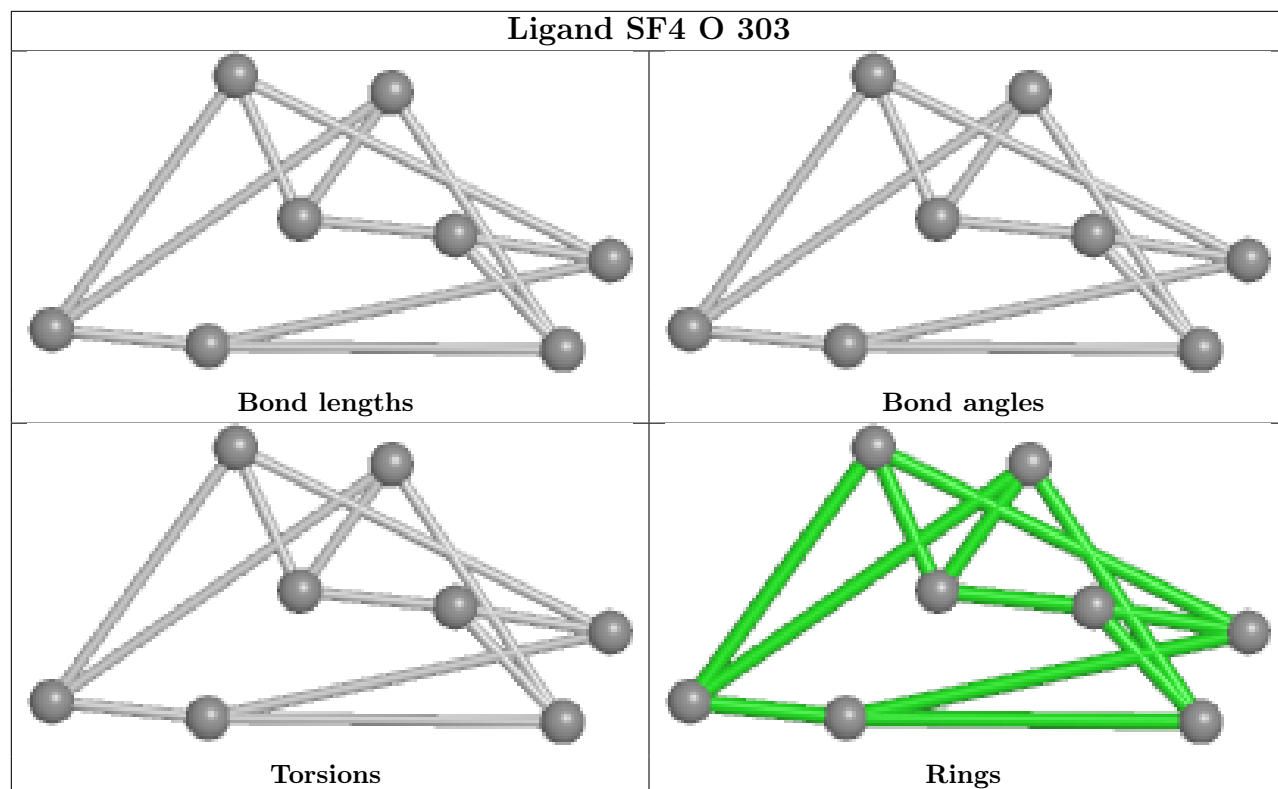
Ligand SF4 I 501



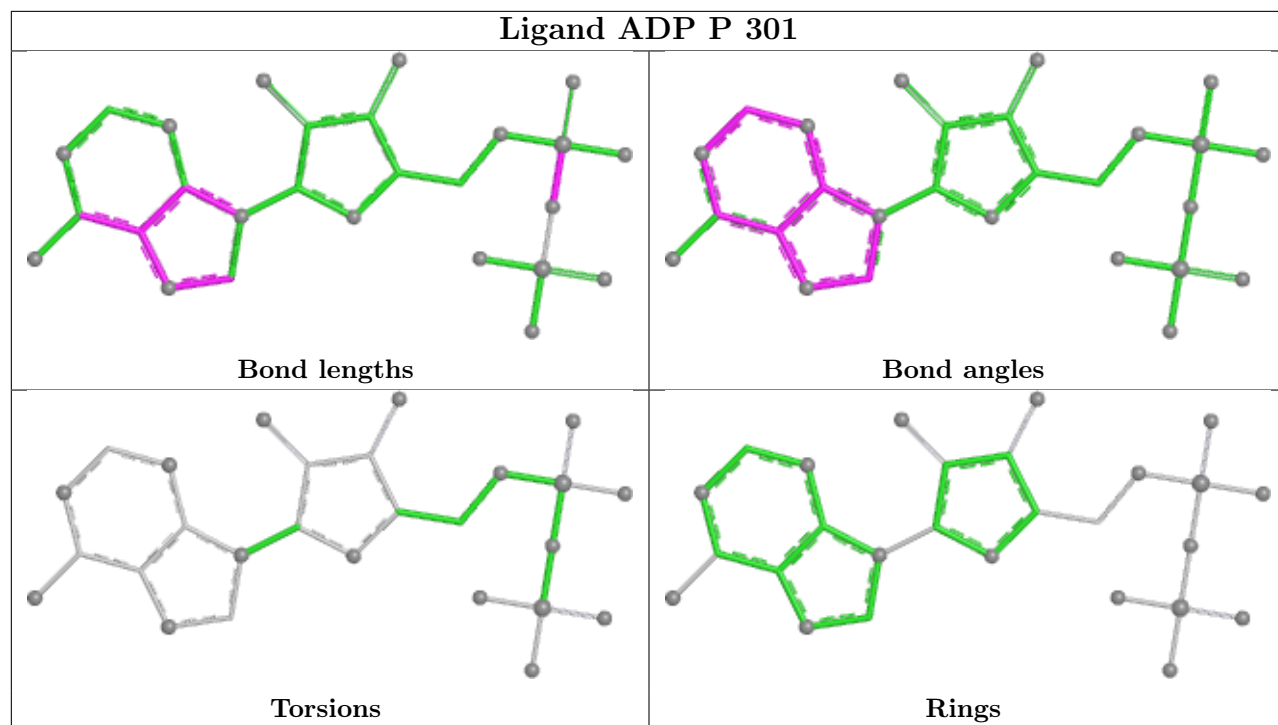
Ligand ATP K 301



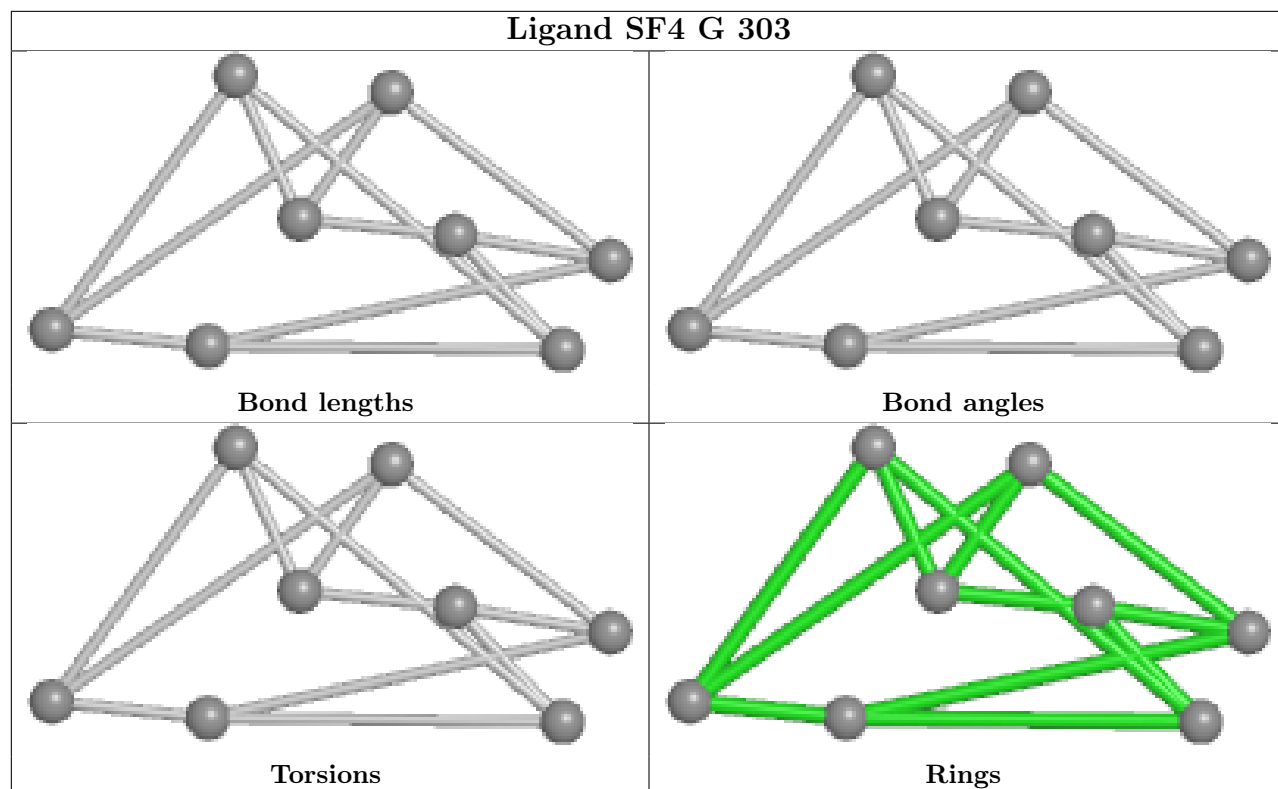
Ligand SF4 O 303



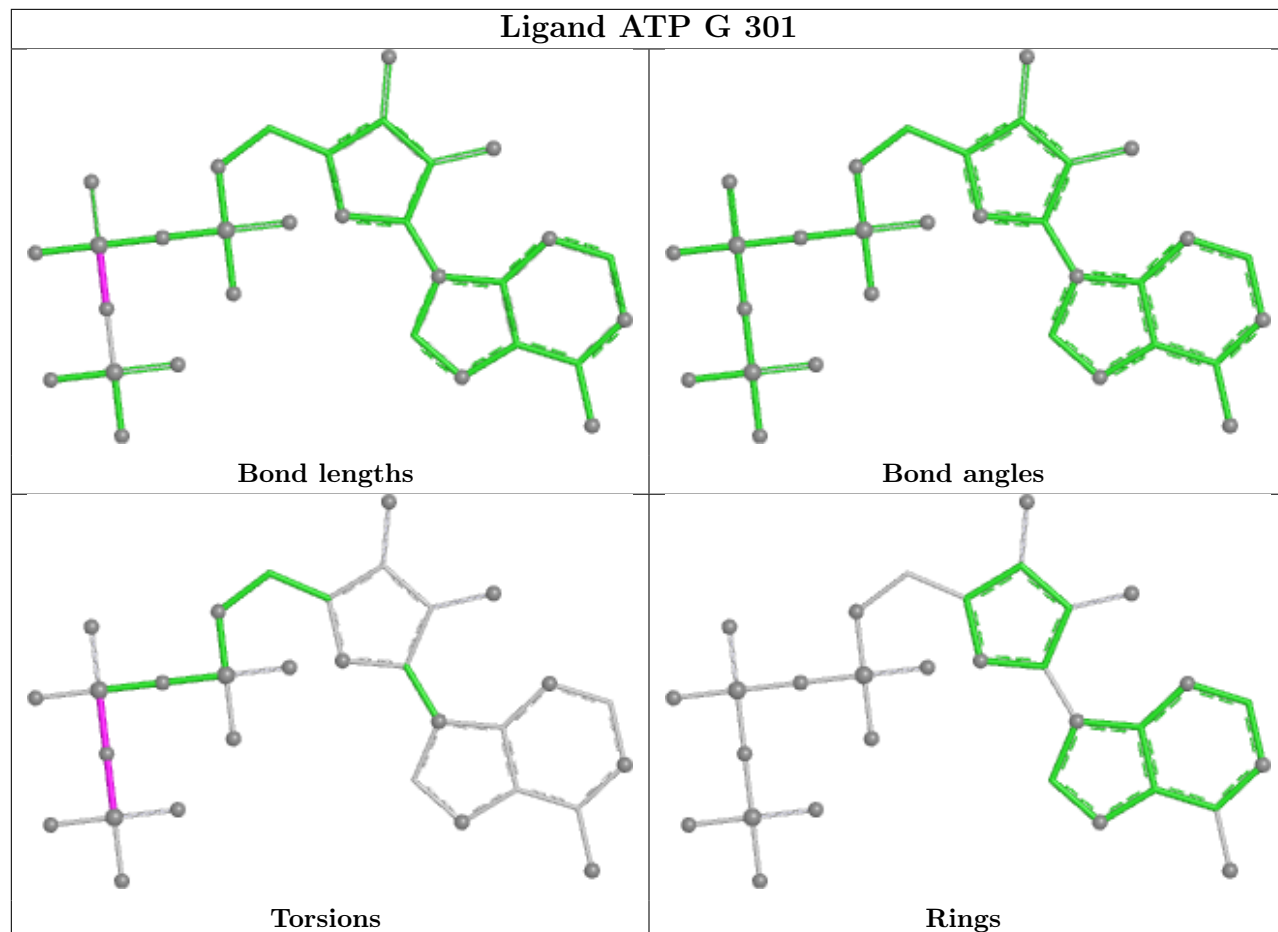
Ligand ADP P 301



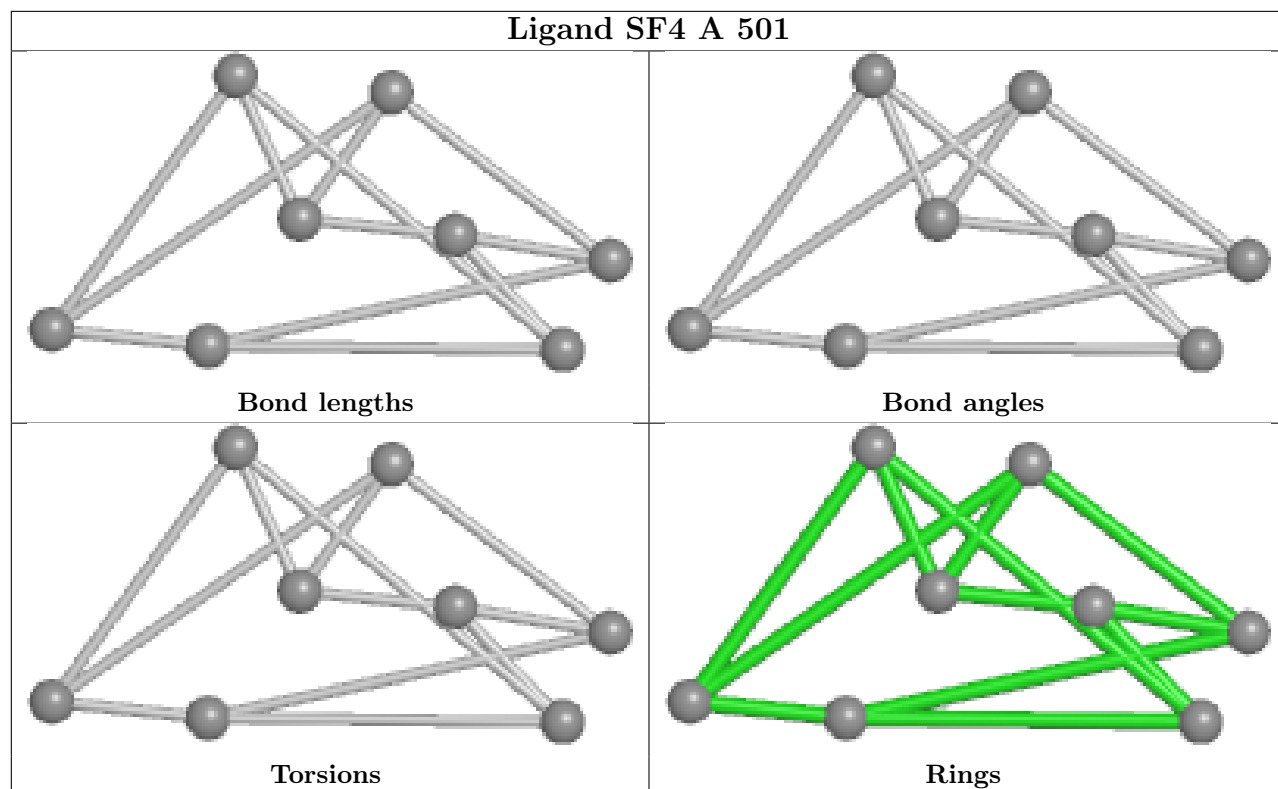
Ligand SF4 G 303



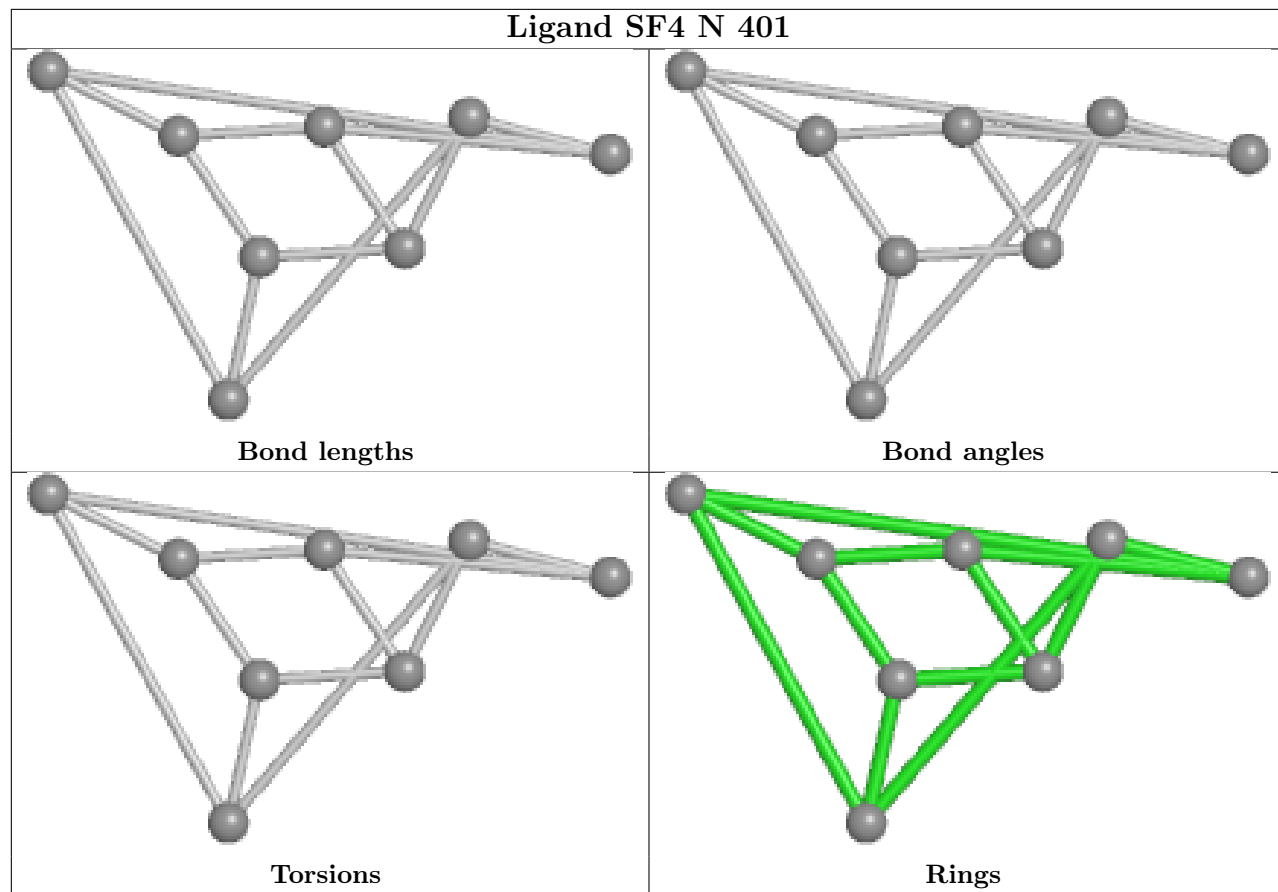
Ligand ATP G 301

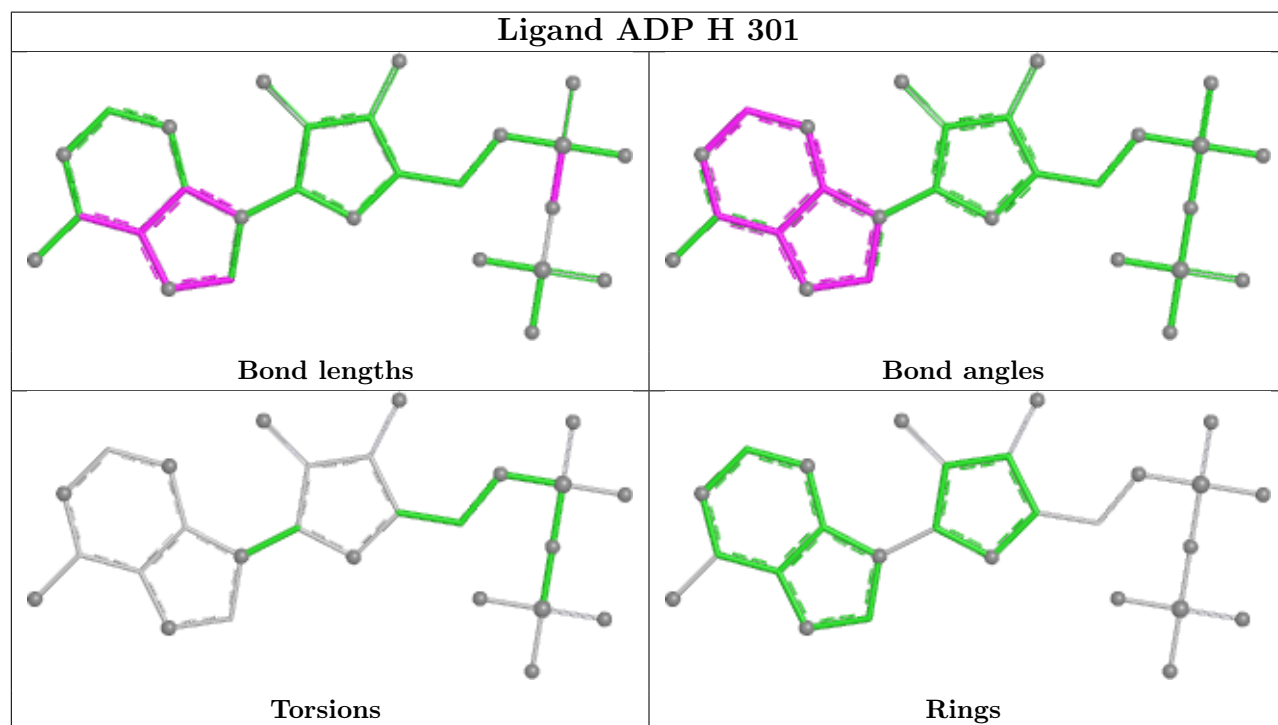
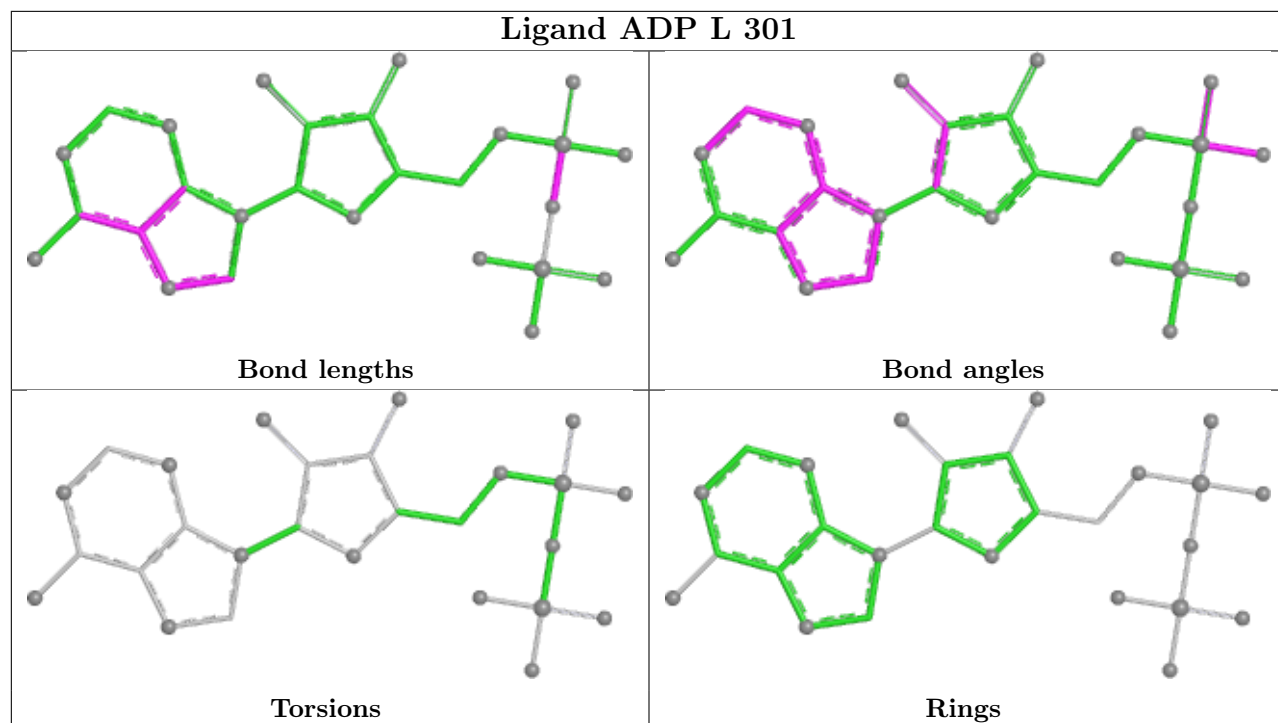


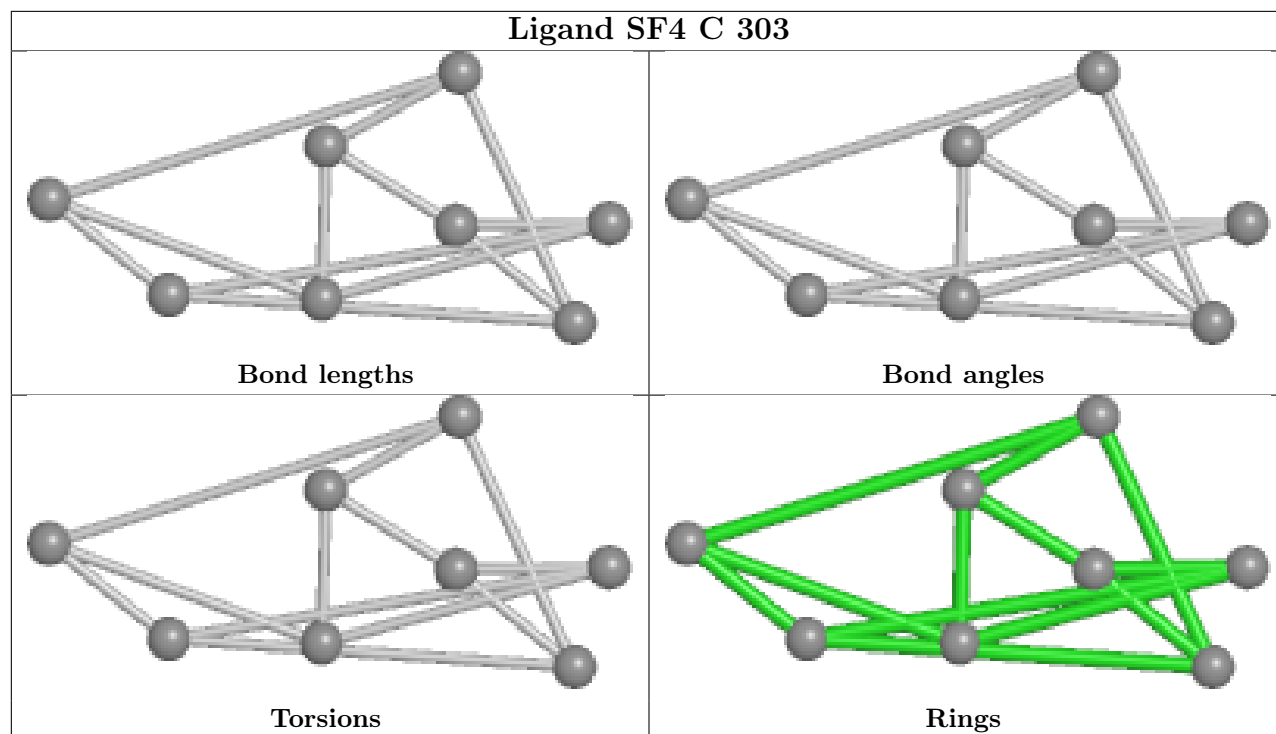
Ligand SF4 A 501



Ligand SF4 N 401







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/445 (98%)	-0.10	12 (2%) 56 60	14, 30, 51, 81	6 (1%)
1	E	436/445 (97%)	-0.04	10 (2%) 61 65	12, 32, 52, 77	3 (0%)
1	I	437/445 (98%)	-0.12	9 (2%) 63 67	12, 30, 47, 74	2 (0%)
1	M	437/445 (98%)	-0.10	12 (2%) 56 60	15, 30, 49, 81	3 (0%)
2	B	387/388 (99%)	-0.05	4 (1%) 79 82	16, 35, 53, 74	4 (1%)
2	F	387/388 (99%)	0.02	4 (1%) 79 82	15, 36, 57, 79	2 (0%)
2	J	387/388 (99%)	-0.08	4 (1%) 79 82	16, 33, 51, 70	1 (0%)
2	N	387/388 (99%)	-0.37	5 (1%) 75 78	14, 27, 41, 60	4 (1%)
3	C	264/273 (96%)	0.12	7 (2%) 56 60	15, 35, 54, 68	3 (1%)
3	G	264/273 (96%)	0.08	5 (1%) 66 70	15, 34, 53, 66	3 (1%)
3	K	264/273 (96%)	0.35	10 (3%) 44 47	16, 39, 65, 79	6 (2%)
3	O	265/273 (97%)	0.11	8 (3%) 52 56	14, 34, 49, 62	3 (1%)
4	D	261/269 (97%)	0.20	6 (2%) 61 65	17, 39, 60, 75	4 (1%)
4	H	261/269 (97%)	0.05	3 (1%) 78 80	15, 34, 50, 66	2 (0%)
4	L	261/269 (97%)	0.32	8 (3%) 51 55	16, 41, 61, 68	3 (1%)
4	P	261/269 (97%)	0.14	6 (2%) 61 65	14, 37, 56, 66	1 (0%)
All	All	5396/5500 (98%)	0.00	113 (2%) 63 67	12, 33, 54, 81	50 (0%)

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	442	ALA	5.8
1	M	442	ALA	5.4
2	F	2	ALA	5.1
3	K	234	LEU	4.8
2	F	388	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
3	O	234	LEU	4.7
1	A	75	PHE	4.6
1	I	75	PHE	4.4
3	O	265	GLY	4.4
3	G	67	TYR	4.3
1	I	442	ALA	4.3
2	J	2	ALA	4.1
2	B	388	ASP	4.0
3	O	264	ARG	3.8
1	E	335	ASN	3.7
1	E	7	MET	3.6
3	C	234	LEU	3.6
2	N	2	ALA	3.5
2	B	2	ALA	3.4
4	L	233	GLY	3.4
3	K	141	TYR	3.3
2	B	152[A]	ARG	3.2
1	M	436	SER	3.2
1	A	163[A]	LYS	3.2
1	A	441	GLN	3.1
1	M	75	PHE	3.1
1	M	74	ALA	3.1
1	I	6	GLN	3.1
1	A	7	MET	3.1
1	I	7	MET	3.1
4	H	115	ASN	3.0
4	D	184[A]	VAL	3.0
4	L	67	TYR	3.0
1	E	6	GLN	3.0
2	J	360	PHE	3.0
4	P	106	ASP	2.9
3	G	119[A]	ARG	2.9
3	G	234	LEU	2.9
1	A	318	TYR	2.8
1	A	74	ALA	2.8
1	M	114[A]	MET	2.8
1	A	6	GLN	2.8
3	O	141	TYR	2.8
1	E	75	PHE	2.8
3	K	264	ARG	2.8
3	C	1	MET	2.8
2	N	74[A]	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	147	ALA	2.7
1	I	26	PHE	2.7
4	H	67	TYR	2.7
4	D	261	GLY	2.7
2	J	74	ASN	2.7
4	L	115	ASN	2.7
2	N	388	ASP	2.6
3	K	140[A]	ARG	2.6
3	K	232	LEU	2.6
4	D	115	ASN	2.6
4	L	261	GLY	2.6
1	M	6	GLN	2.6
2	F	385	ILE	2.6
1	I	74	ALA	2.6
3	O	232	LEU	2.5
1	M	276	THR	2.5
1	M	7	MET	2.5
3	G	264	ARG	2.5
1	E	318	TYR	2.5
2	N	163	GLY	2.5
3	O	233	ASN	2.5
4	D	205[A]	ARG	2.5
1	E	441	GLN	2.4
3	K	1	MET	2.4
4	L	200[A]	ILE	2.4
1	A	8	THR	2.4
4	P	261	GLY	2.4
3	G	1	MET	2.4
2	F	166	ILE	2.3
4	H	261	GLY	2.3
2	B	381	PHE	2.3
2	J	381	PHE	2.3
1	I	335	ASN	2.3
1	I	114	MET	2.3
3	C	54	ILE	2.3
1	I	283	LYS	2.3
3	C	197	LYS	2.3
1	M	438	ARG	2.2
4	L	208	ILE	2.2
1	M	26	PHE	2.2
1	A	437	ARG	2.2
1	E	437	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
3	O	158	GLU	2.2
1	M	441	GLN	2.2
4	P	140	ASP	2.2
1	E	11	GLY	2.2
1	M	76	ARG	2.2
3	K	122[A]	ARG	2.2
1	A	276	THR	2.1
4	P	55	LYS	2.1
3	K	131	THR	2.1
3	O	1	MET	2.1
1	E	439	GLN	2.1
4	P	141	ALA	2.1
3	C	144	TYR	2.1
4	P	115	ASN	2.1
4	L	158	LYS	2.0
1	A	165	GLY	2.0
1	E	167	GLN	2.0
3	C	232	LEU	2.0
4	L	141	ALA	2.0
3	K	145[A]	ASP	2.0
4	D	56	ARG	2.0
3	K	207	ASN	2.0
4	D	116	GLY	2.0
2	N	323[A]	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	GOL	I	504	6/6	0.74	0.19	44,46,47,51	0
7	GOL	A	505	6/6	0.81	0.17	34,45,48,60	0
7	GOL	N	403	6/6	0.87	0.13	25,33,45,51	0
7	GOL	A	504	6/6	0.88	0.14	39,46,47,49	0
7	GOL	E	505	6/6	0.88	0.14	37,41,45,45	0
7	GOL	M	505	6/6	0.91	0.12	37,39,43,47	0
8	K	O	304	1/1	0.93	0.14	63,63,63,63	0
8	K	A	506	1/1	0.96	0.14	54,54,54,54	0
8	K	B	403	1/1	0.96	0.12	45,45,45,45	0
6	CL	E	503	1/1	0.96	0.11	44,44,44,44	0
9	MG	E	502	1/1	0.96	0.06	40,40,40,40	0
6	CL	I	502	1/1	0.97	0.08	43,43,43,43	0
8	K	P	303	1/1	0.97	0.05	45,45,45,45	0
9	MG	B	402	1/1	0.97	0.10	28,28,28,28	0
6	CL	J	402	1/1	0.97	0.10	40,40,40,40	0
9	MG	H	303	1/1	0.97	0.07	27,27,27,27	0
9	MG	L	303	1/1	0.97	0.07	32,32,32,32	0
8	K	F	404	1/1	0.98	0.12	44,44,44,44	0
8	K	J	403	1/1	0.98	0.15	43,43,43,43	0
8	K	J	404	1/1	0.98	0.10	38,38,38,38	0
8	K	N	404	1/1	0.98	0.16	38,38,38,38	0
7	GOL	A	503	6/6	0.98	0.04	20,23,24,27	0
7	GOL	M	504	6/6	0.98	0.05	22,25,25,28	0
6	CL	A	502	1/1	0.98	0.10	46,46,46,46	0
6	CL	F	403	1/1	0.98	0.16	43,43,43,43	0
6	CL	M	503	1/1	0.98	0.09	44,44,44,44	0
7	GOL	I	503	6/6	0.98	0.06	22,22,27,27	0
9	MG	M	502	1/1	0.98	0.06	32,32,32,32	0
10	ATP	K	301	31/31	0.98	0.05	28,37,44,47	0
10	ATP	O	301	31/31	0.98	0.05	23,32,38,41	0
11	ADP	D	301	27/27	0.98	0.05	26,30,36,37	0
11	ADP	H	301	27/27	0.98	0.05	22,27,32,32	0
11	ADP	L	301	27/27	0.98	0.05	27,33,40,41	0
11	ADP	P	301	27/27	0.98	0.05	25,29,34,37	0
5	SF4	K	303	8/8	0.99	0.03	25,25,26,27	0
7	GOL	E	504	6/6	0.99	0.04	22,23,25,25	0
5	SF4	M	501	8/8	0.99	0.03	22,24,25,26	0
5	SF4	N	401	8/8	0.99	0.03	21,21,22,22	0
9	MG	D	302	1/1	0.99	0.08	19,19,19,19	0
5	SF4	O	303	8/8	0.99	0.03	24,25,26,26	0
9	MG	F	402	1/1	0.99	0.07	27,27,27,27	0
9	MG	G	302	1/1	0.99	0.03	24,24,24,24	0
9	MG	H	302	1/1	0.99	0.09	16,16,16,16	0

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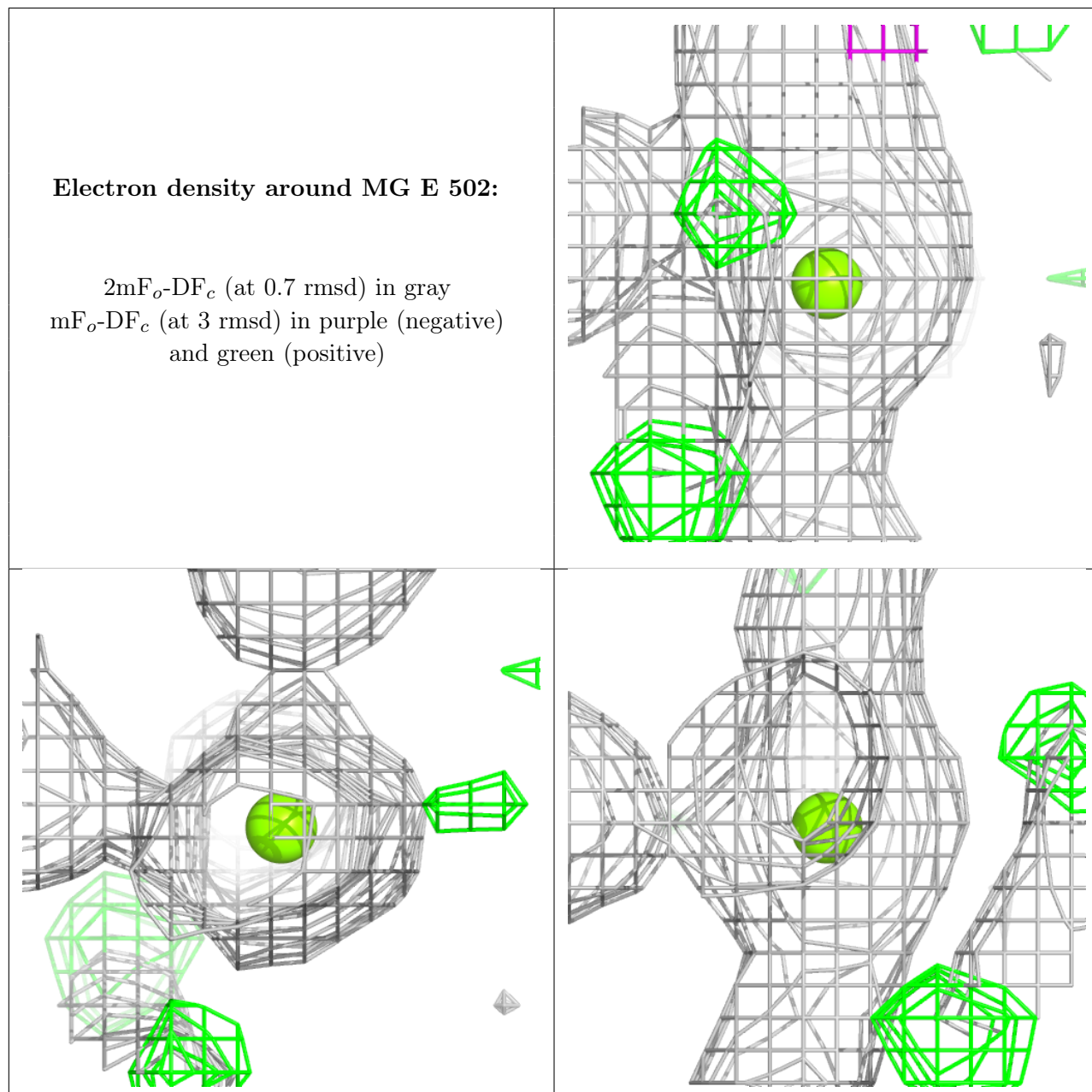
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SF4	A	501	8/8	0.99	0.02	23,24,26,27	0
5	SF4	B	401	8/8	0.99	0.03	24,24,25,26	0
5	SF4	C	303	8/8	0.99	0.03	25,26,26,28	0
9	MG	N	402	1/1	0.99	0.06	25,25,25,25	0
9	MG	O	302	1/1	0.99	0.05	23,23,23,23	0
10	ATP	C	301	31/31	0.99	0.05	23,30,37,37	0
10	ATP	G	301	31/31	0.99	0.05	26,30,34,37	0
5	SF4	E	501	8/8	0.99	0.03	23,25,26,27	0
5	SF4	F	401	8/8	0.99	0.02	24,25,26,26	0
5	SF4	G	303	8/8	0.99	0.03	25,25,26,26	0
5	SF4	I	501	8/8	0.99	0.03	22,25,26,26	0
5	SF4	J	401	8/8	0.99	0.03	23,24,25,25	0
8	K	J	405	1/1	0.99	0.12	40,40,40,40	0
9	MG	K	302	1/1	1.00	0.04	27,27,27,27	0
9	MG	L	302	1/1	1.00	0.10	20,20,20,20	0
9	MG	C	302	1/1	1.00	0.04	23,23,23,23	0
9	MG	P	302	1/1	1.00	0.10	18,18,18,18	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

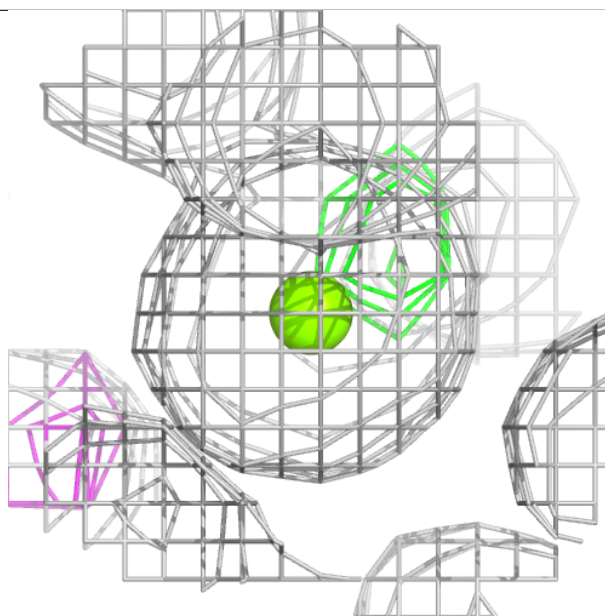
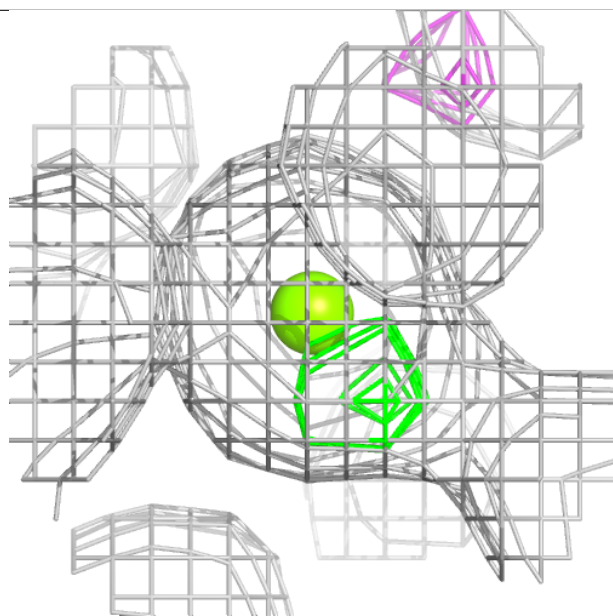
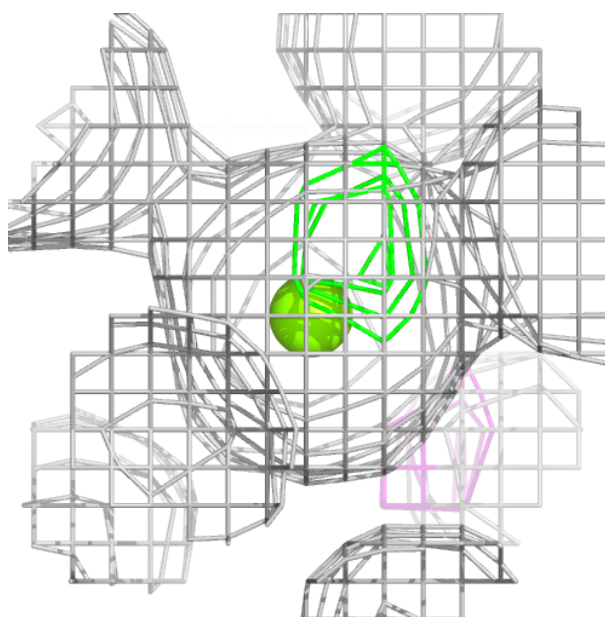
Electron density around MG E 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



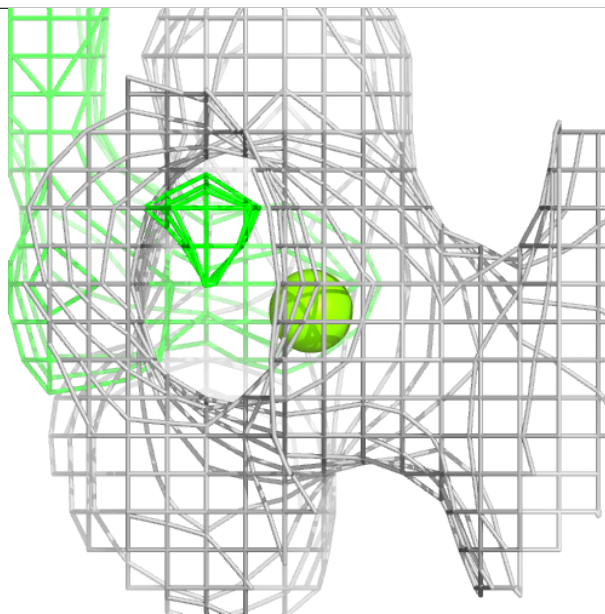
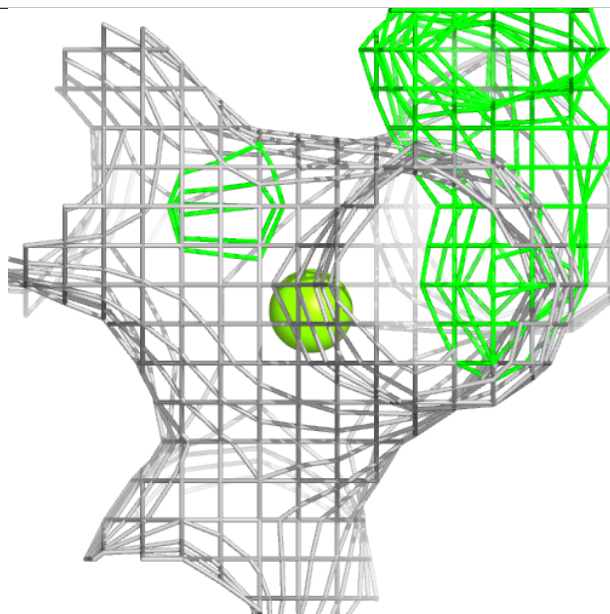
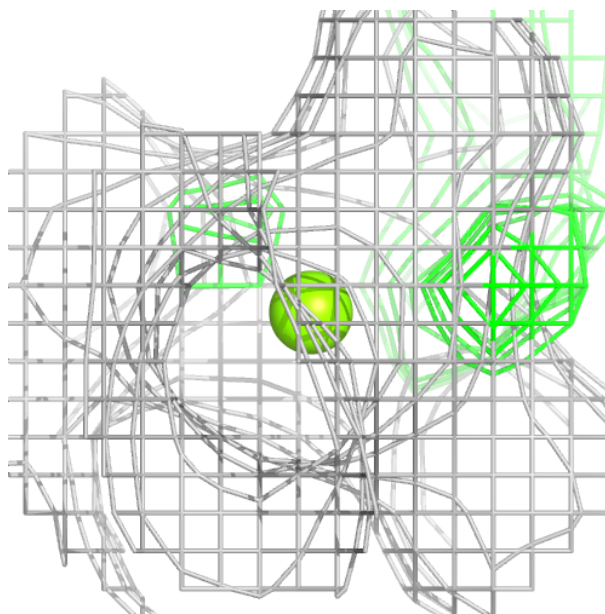
Electron density around MG B 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



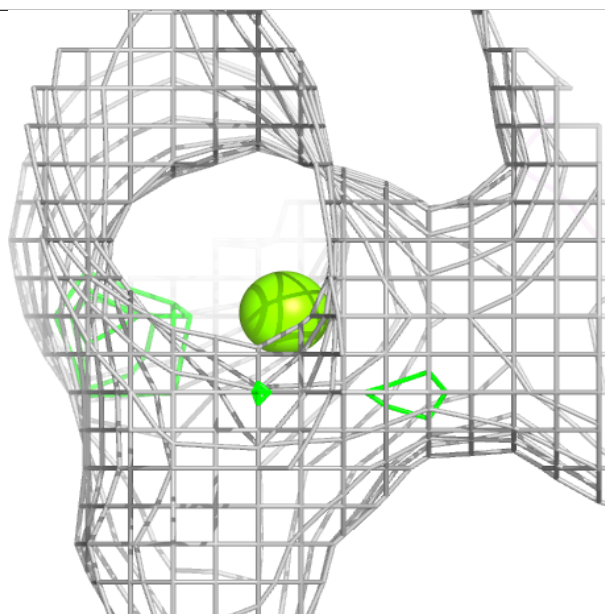
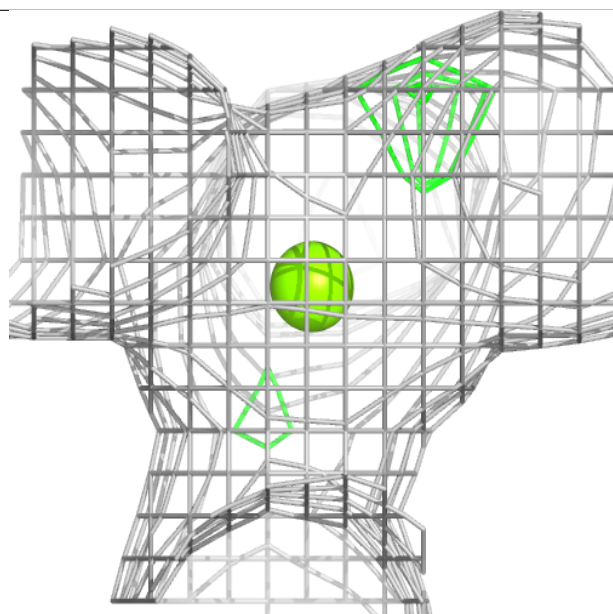
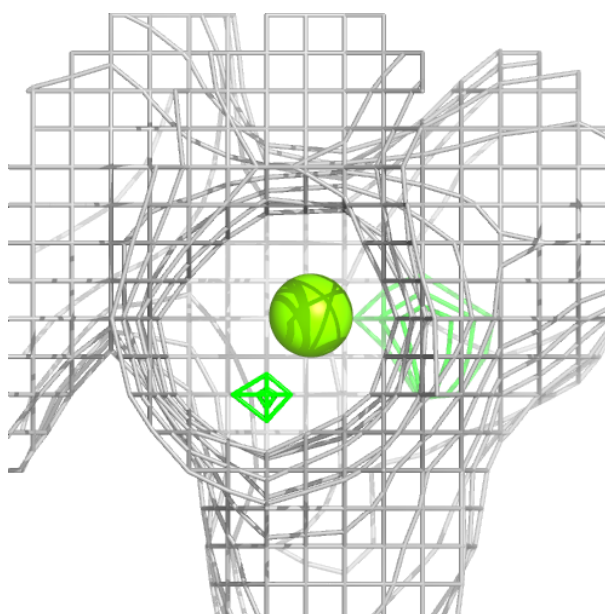
Electron density around MG H 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



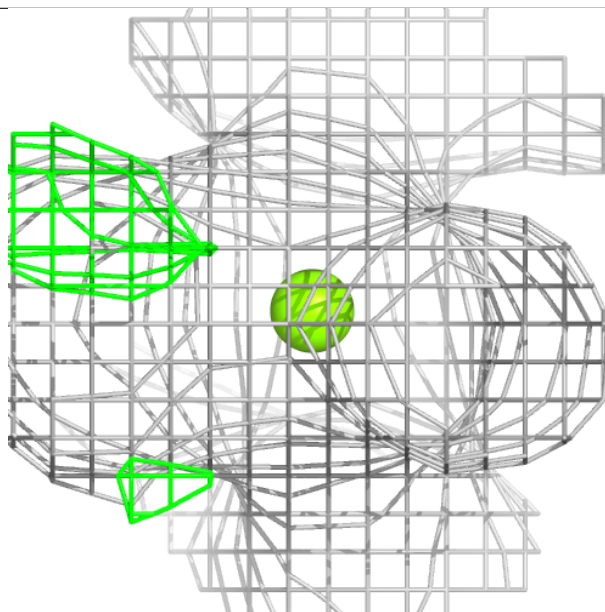
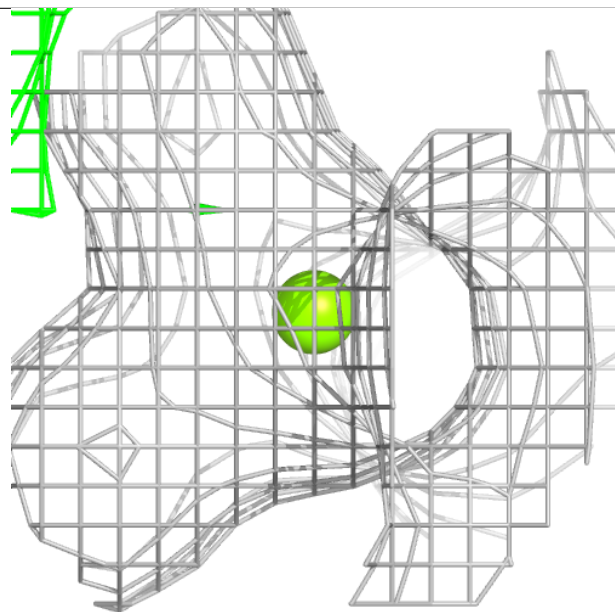
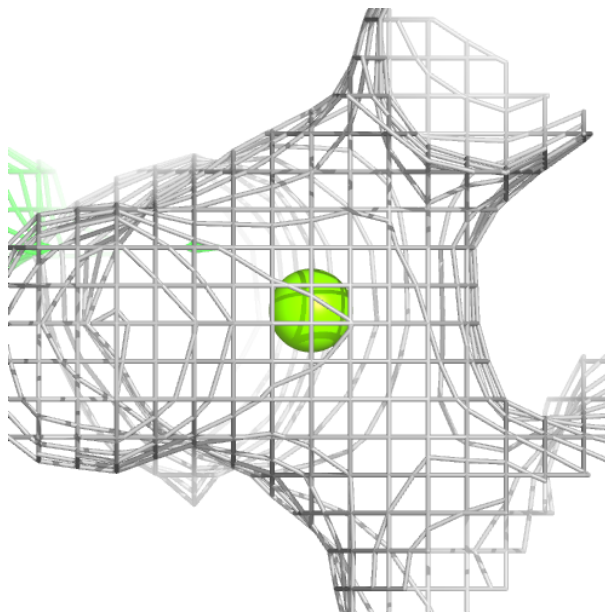
Electron density around MG L 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



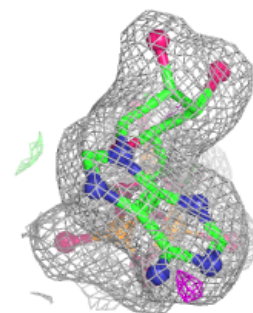
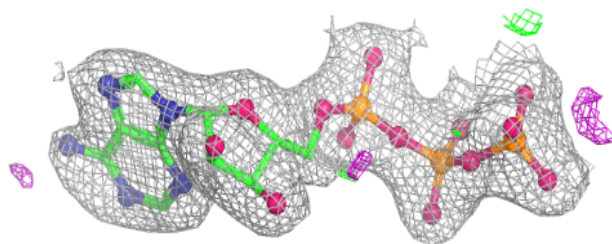
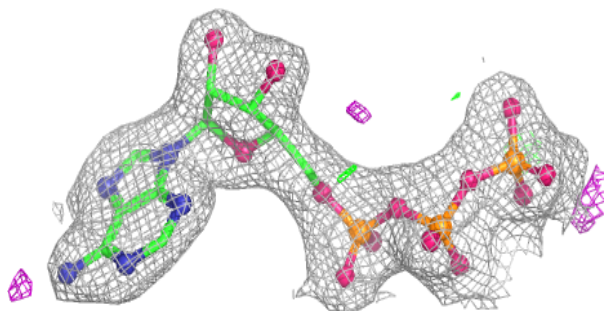
Electron density around MG M 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

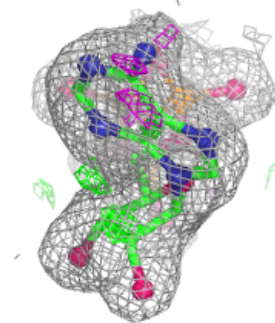
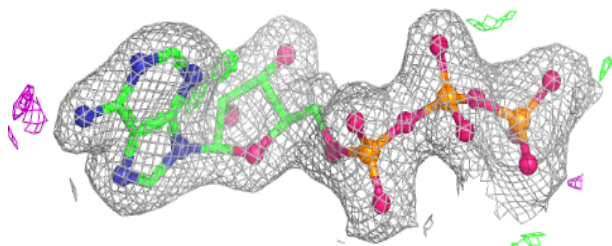
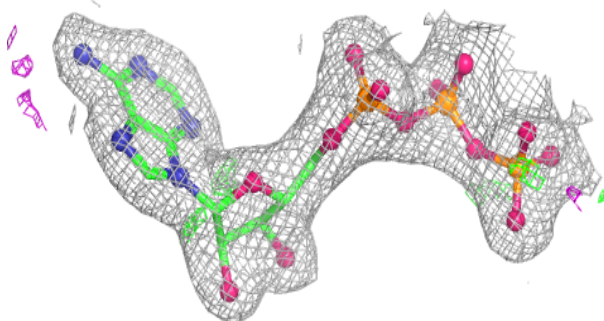


Electron density around ATP K 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

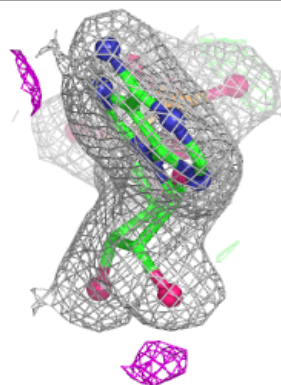
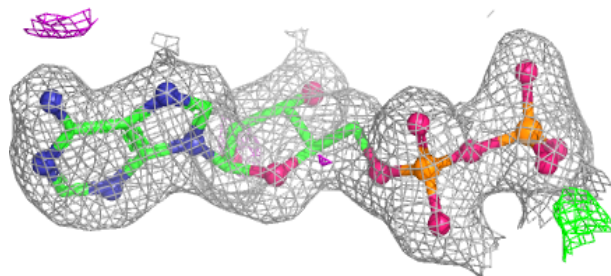
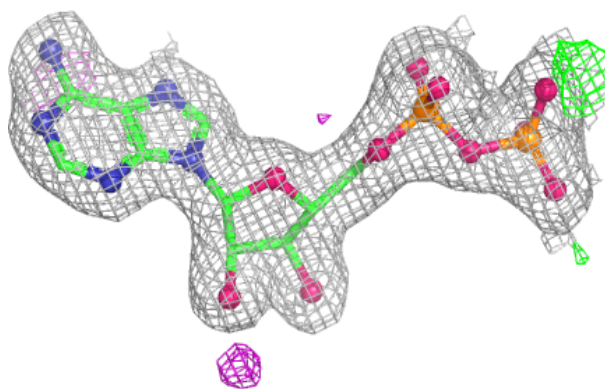
**Electron density around ATP O 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

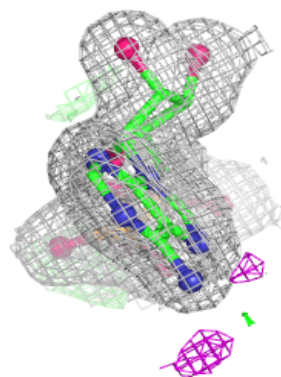
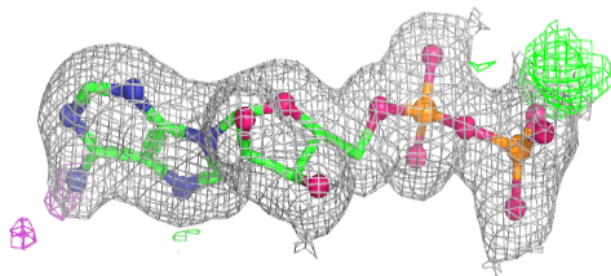
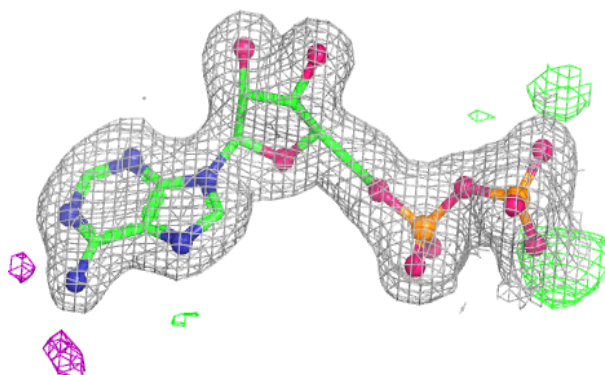


Electron density around ADP D 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

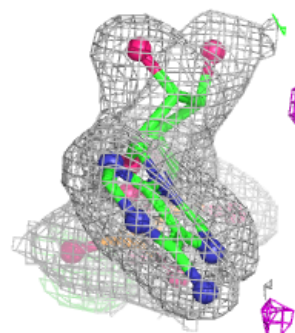
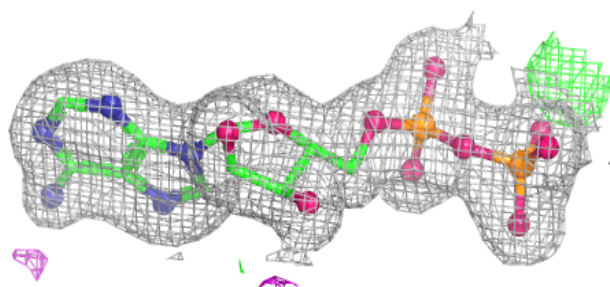
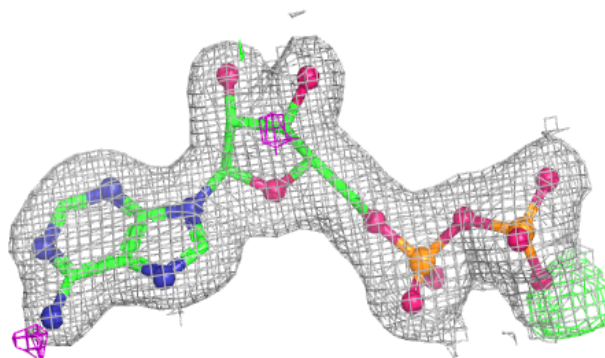
**Electron density around ADP H 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

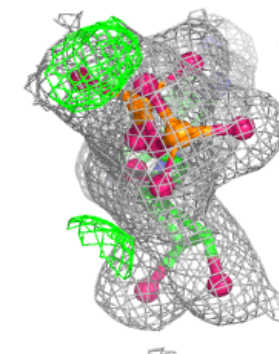
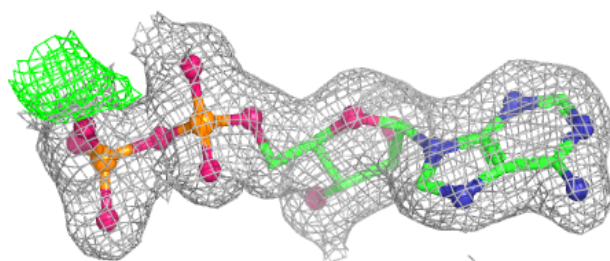
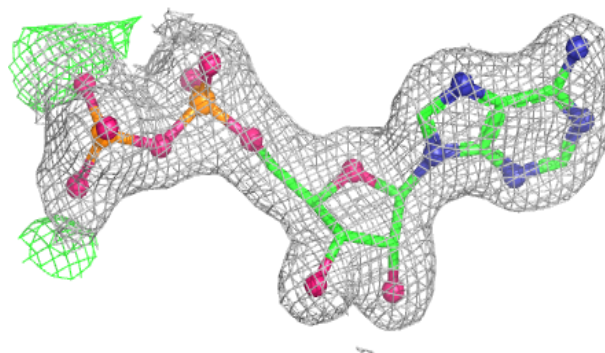


Electron density around ADP L 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

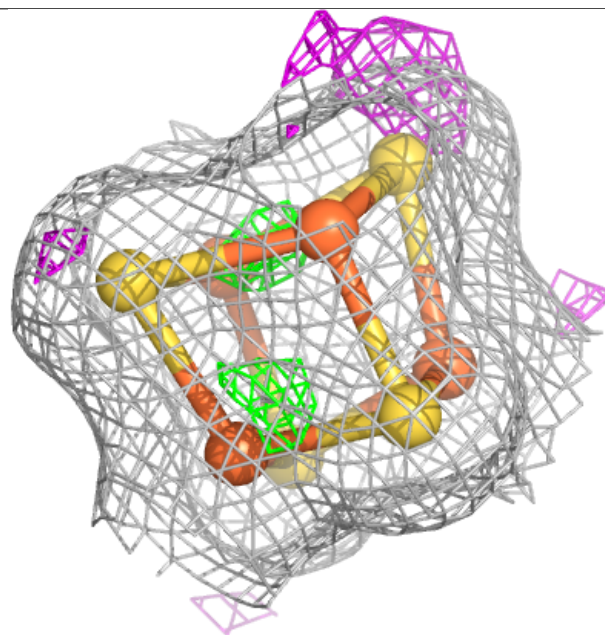
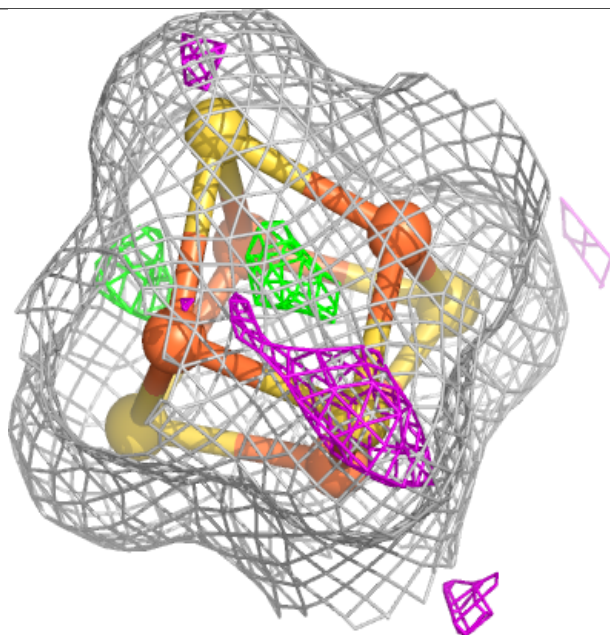
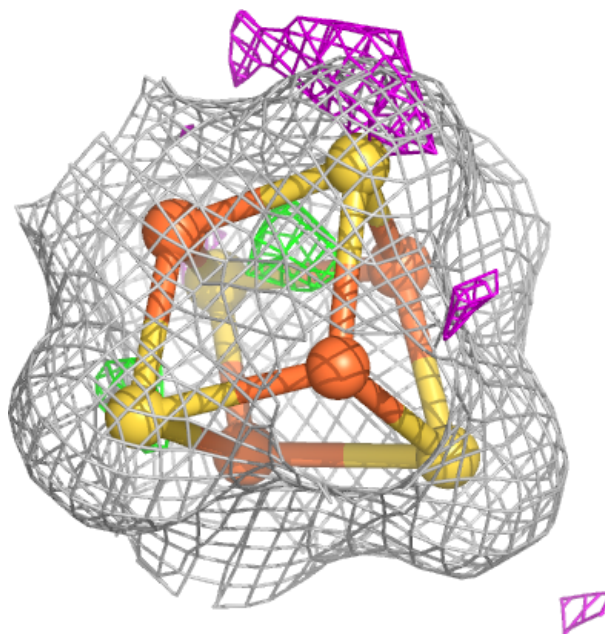
**Electron density around ADP P 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



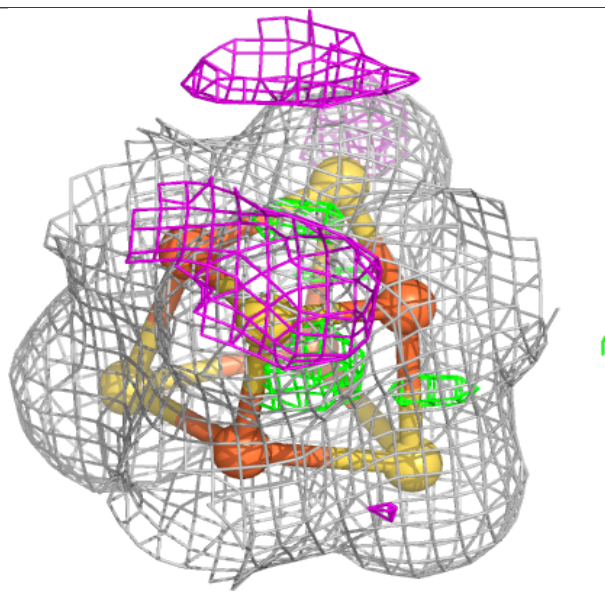
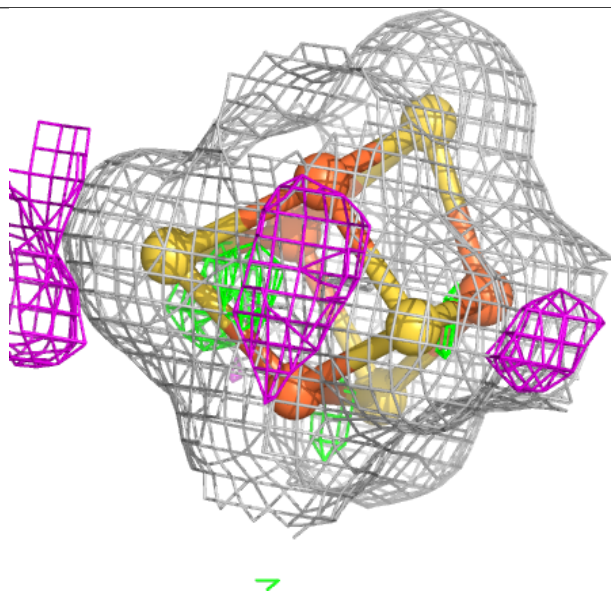
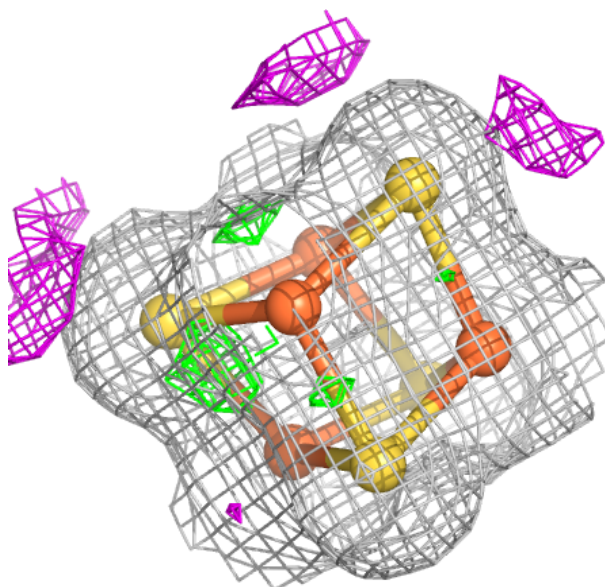
Electron density around SF4 K 303:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



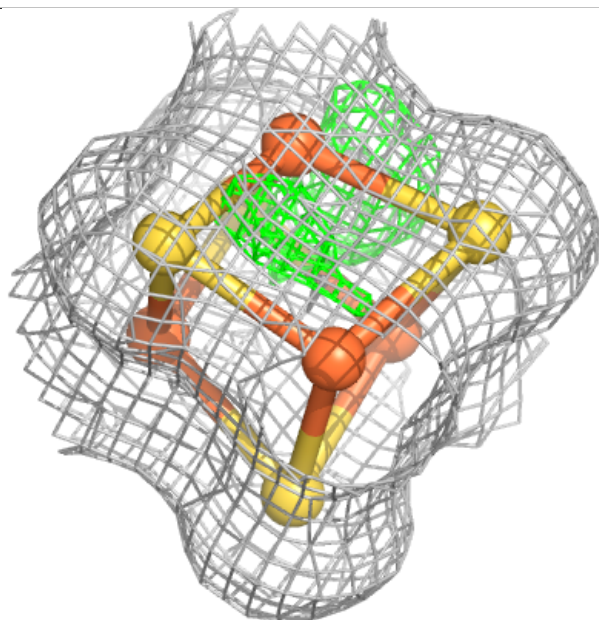
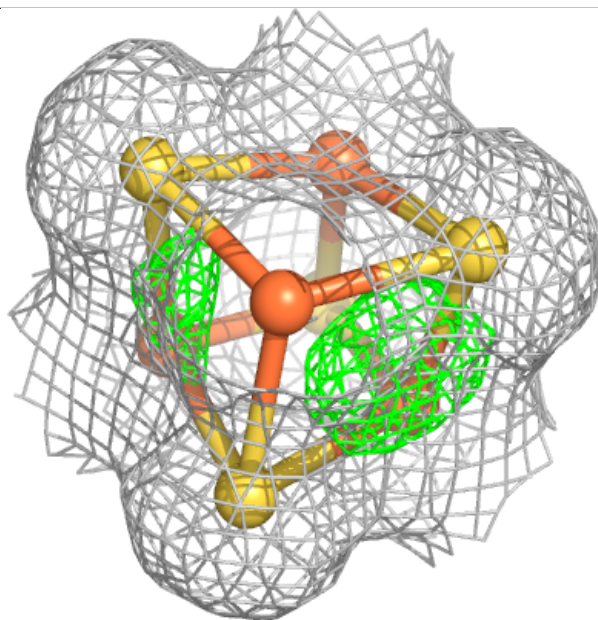
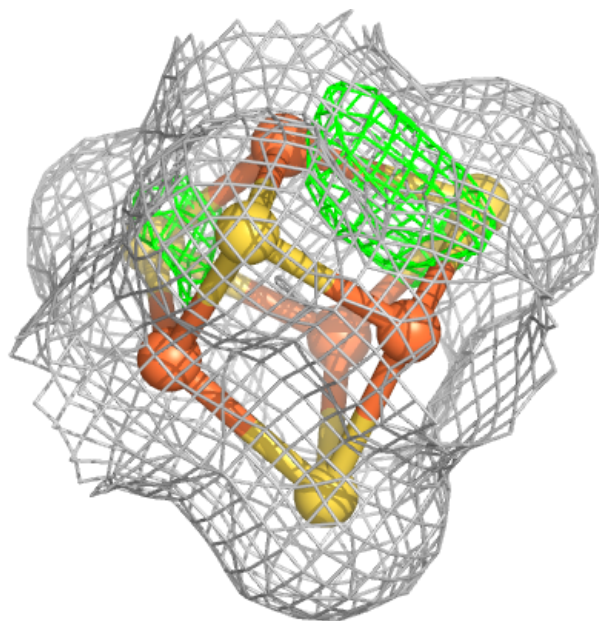
Electron density around SF4 M 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



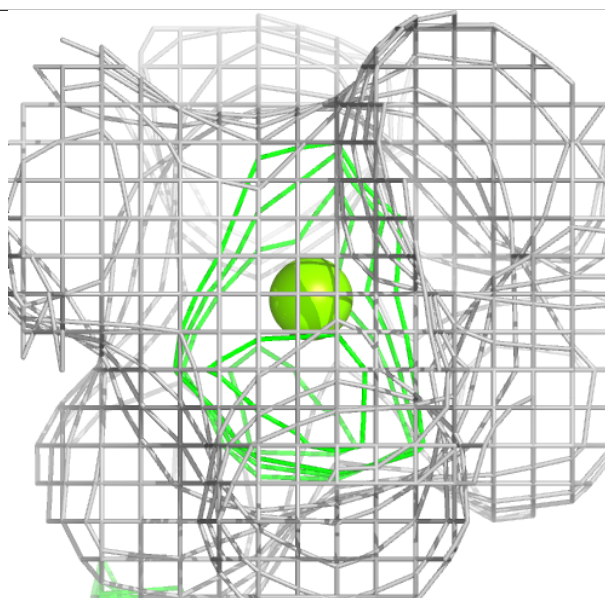
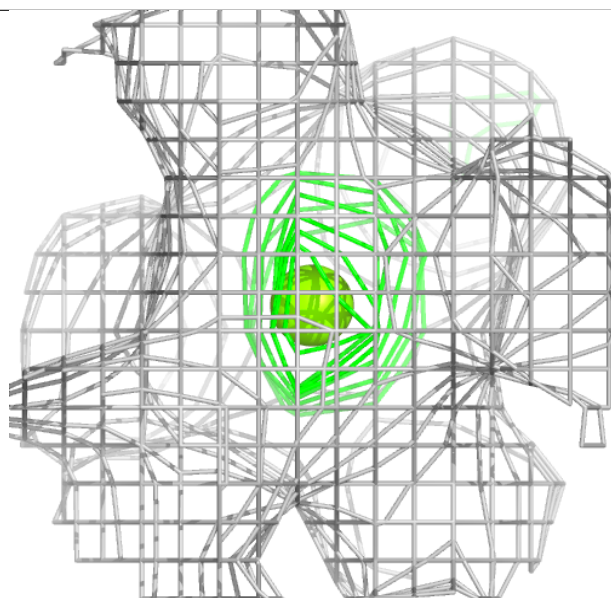
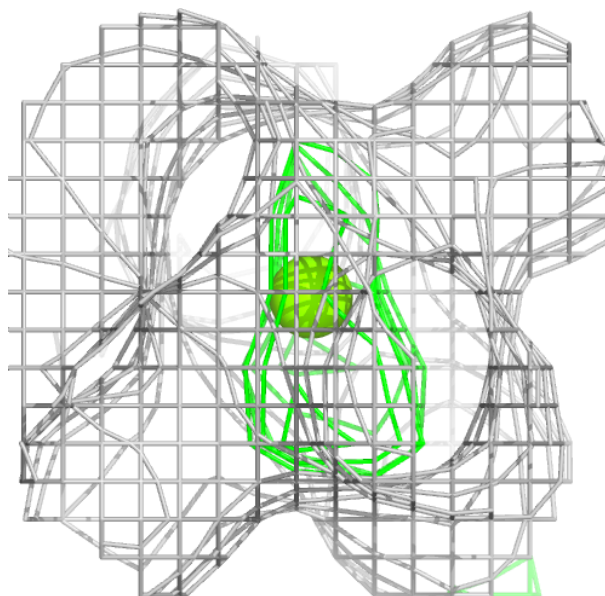
Electron density around SF4 N 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



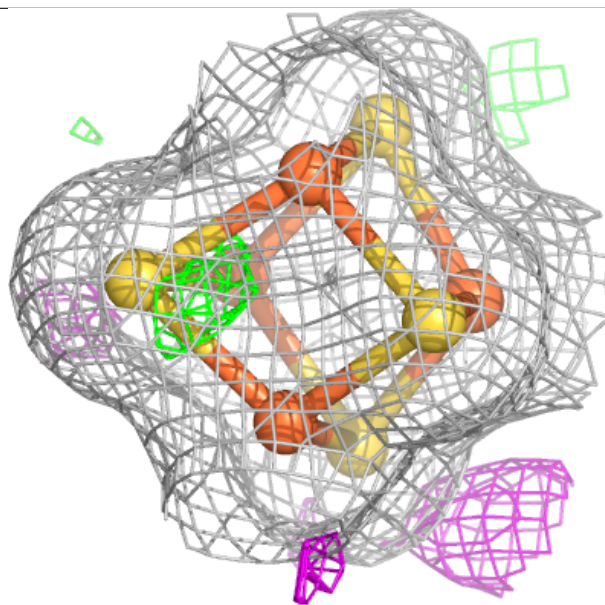
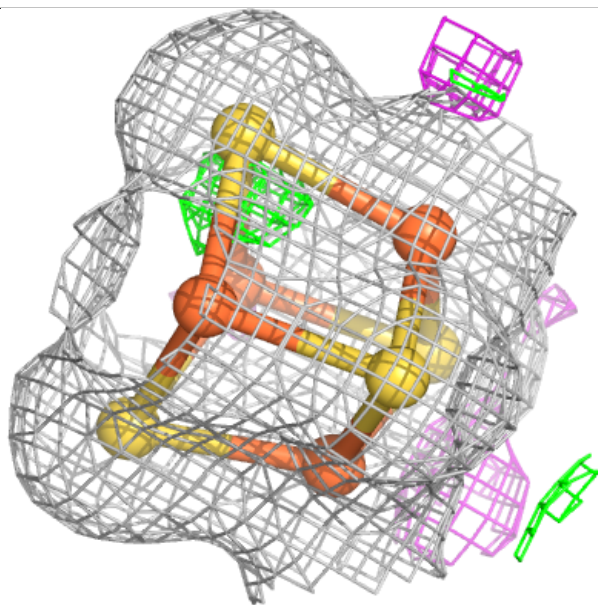
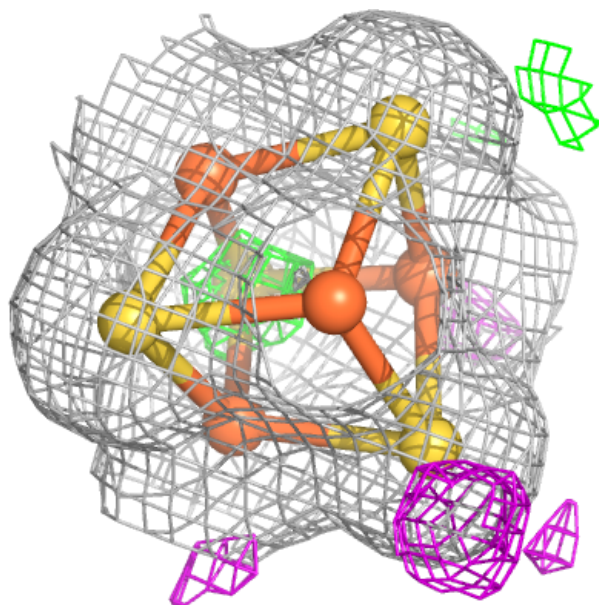
Electron density around MG D 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



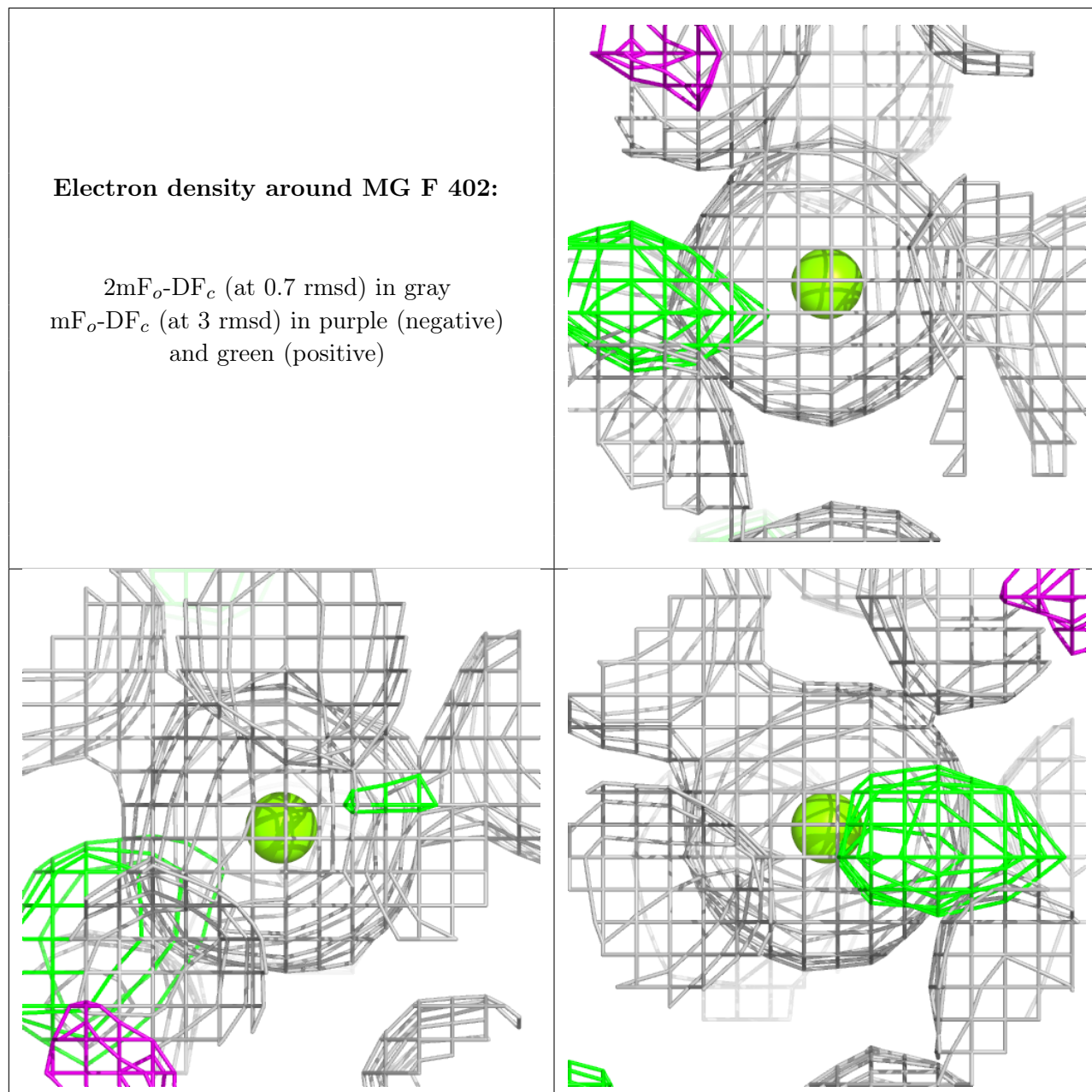
Electron density around SF4 O 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



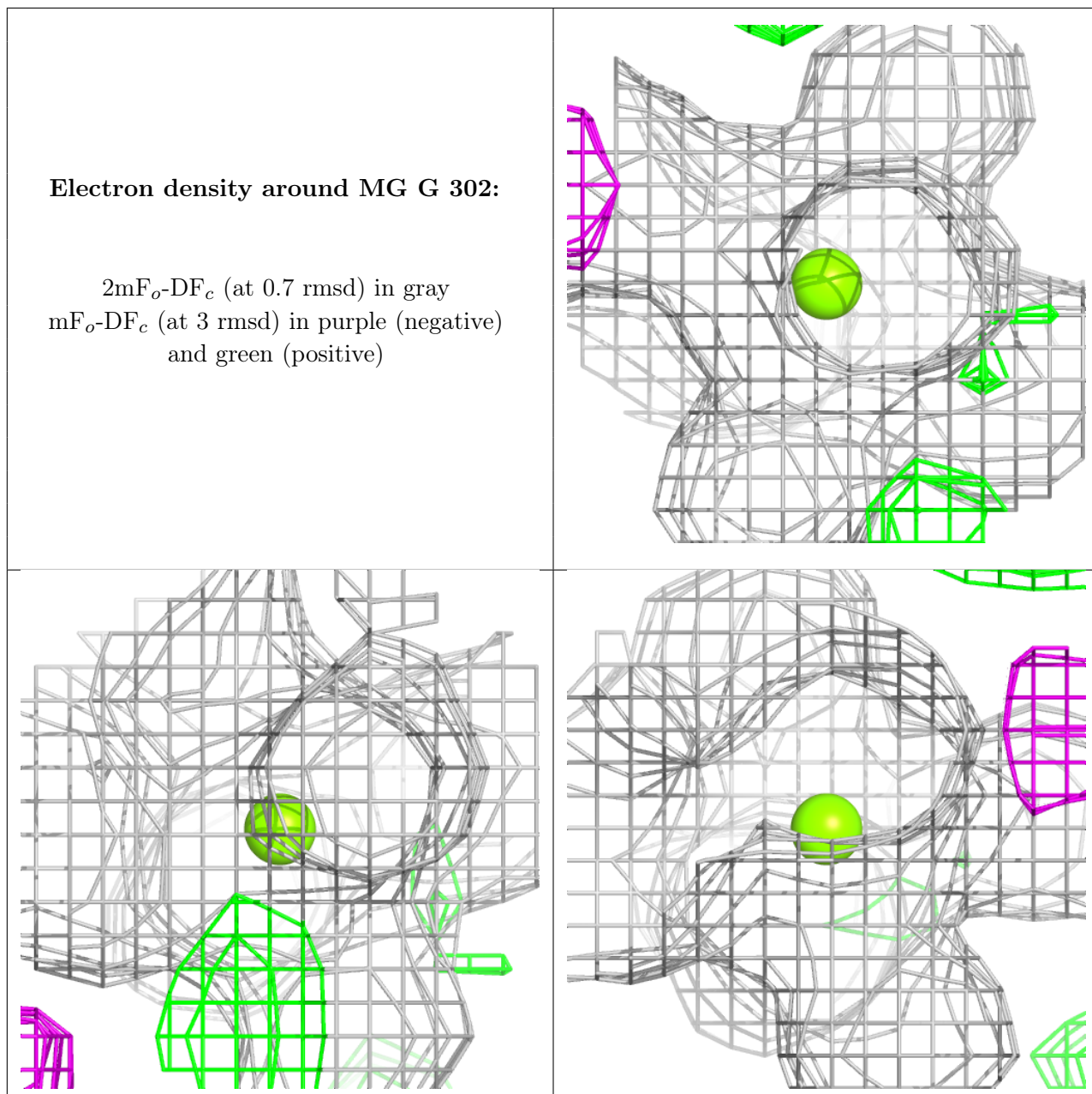
Electron density around MG F 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



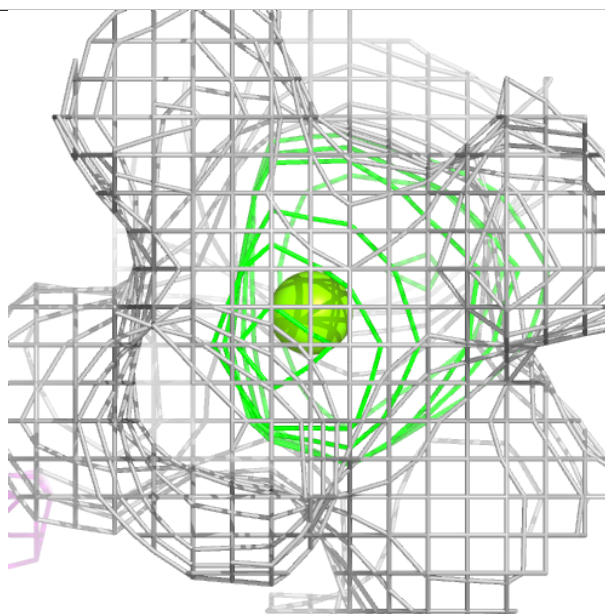
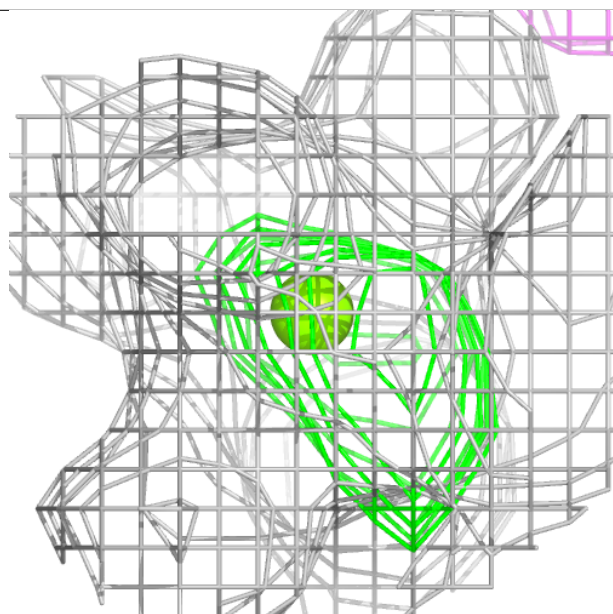
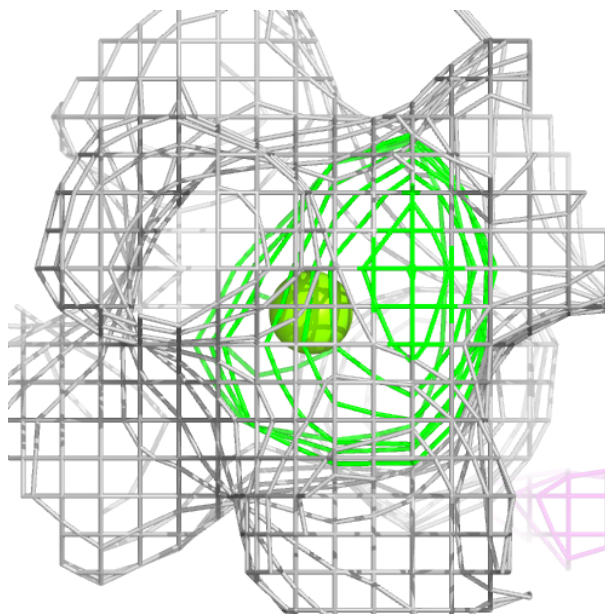
Electron density around MG G 302:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



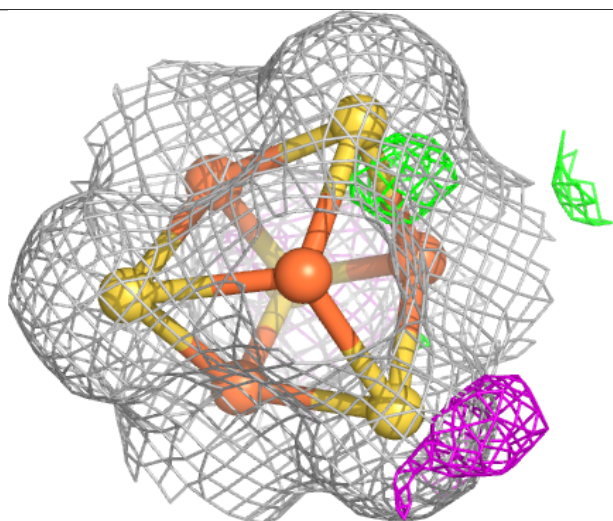
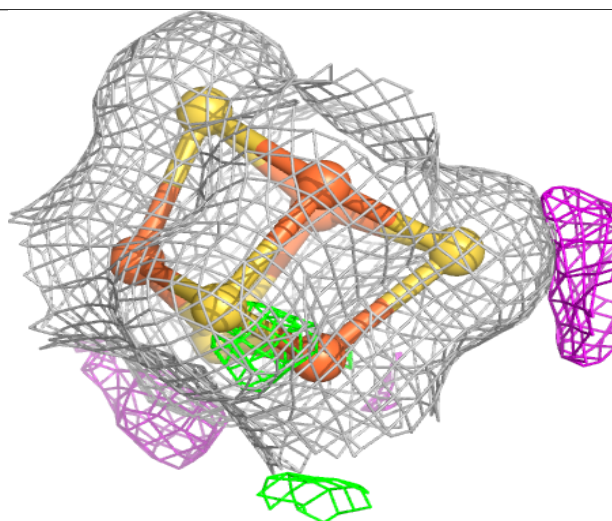
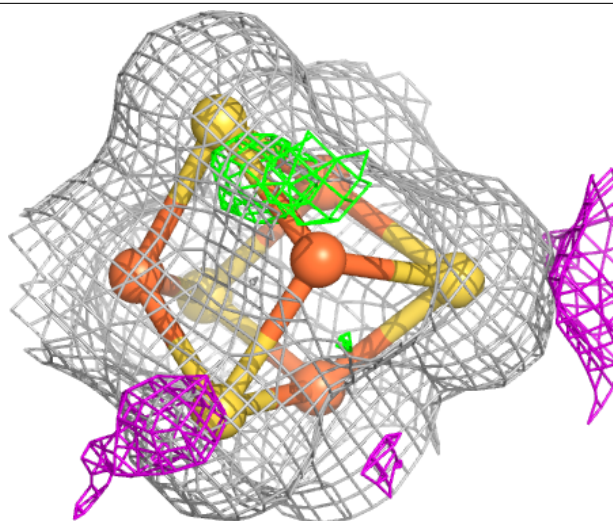
Electron density around MG H 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



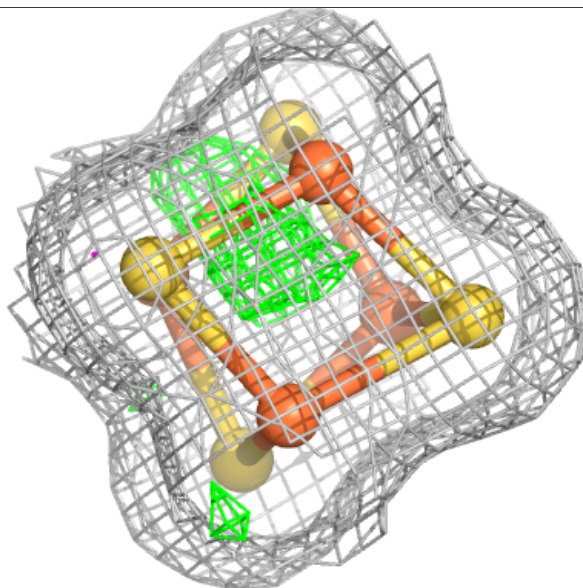
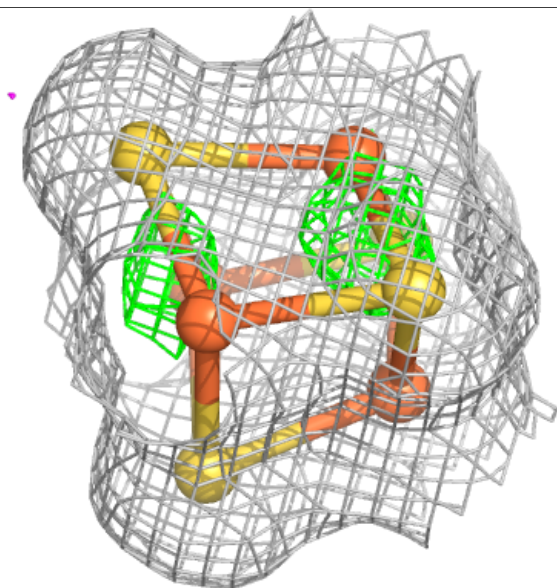
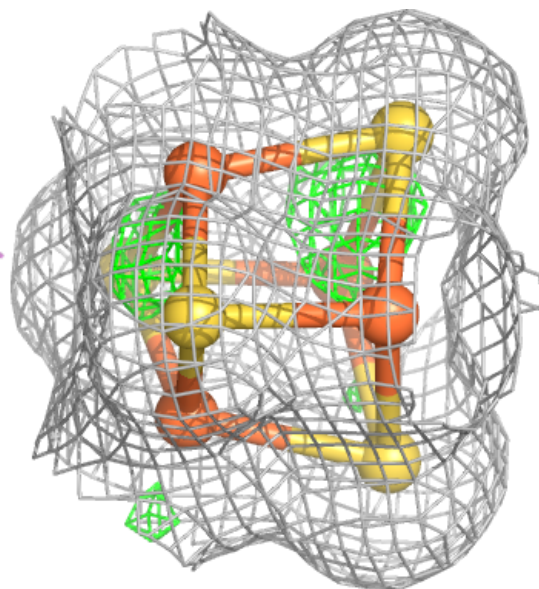
Electron density around SF4 A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



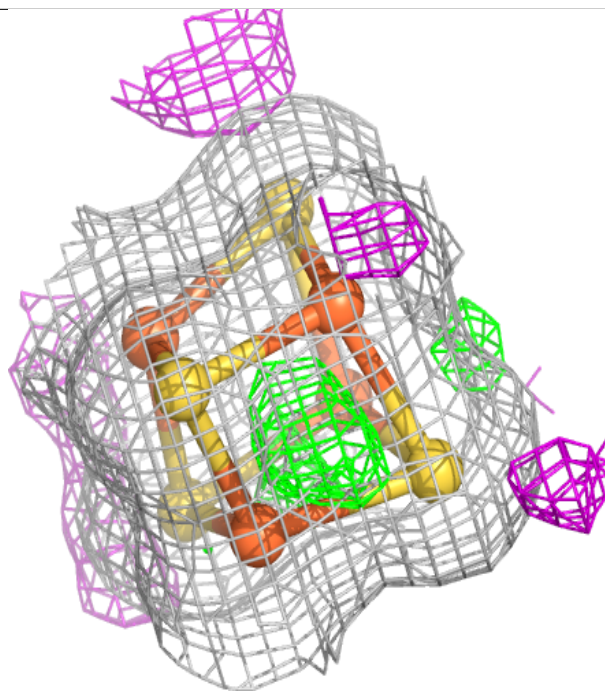
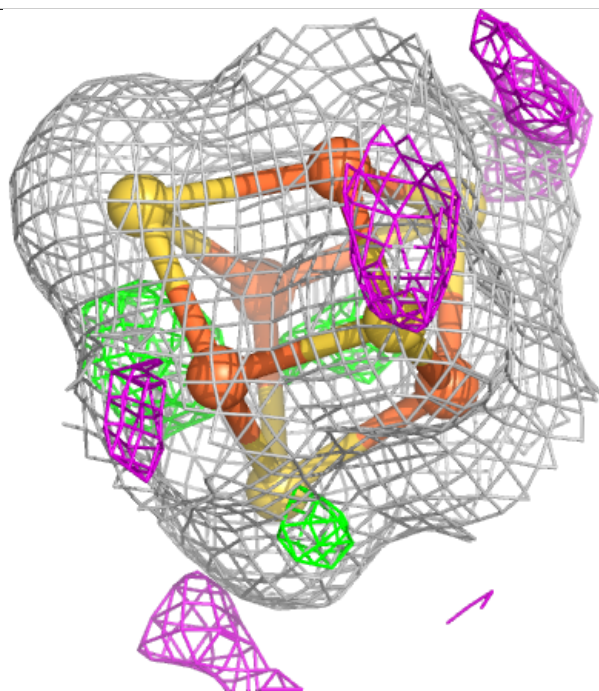
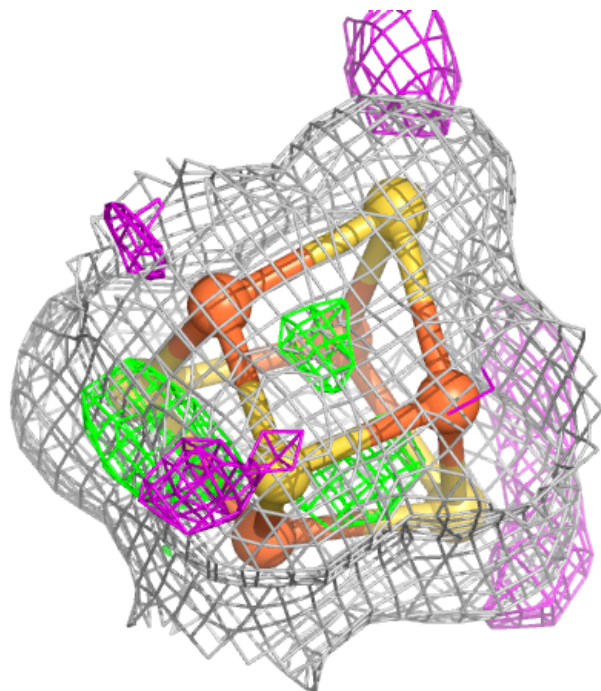
Electron density around SF4 B 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



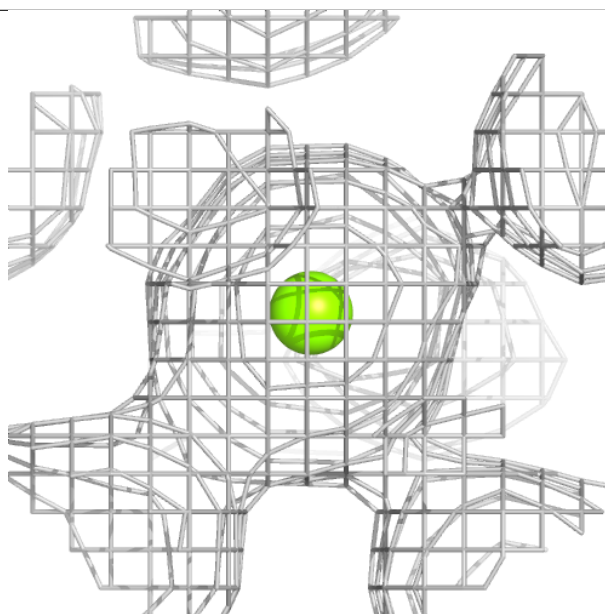
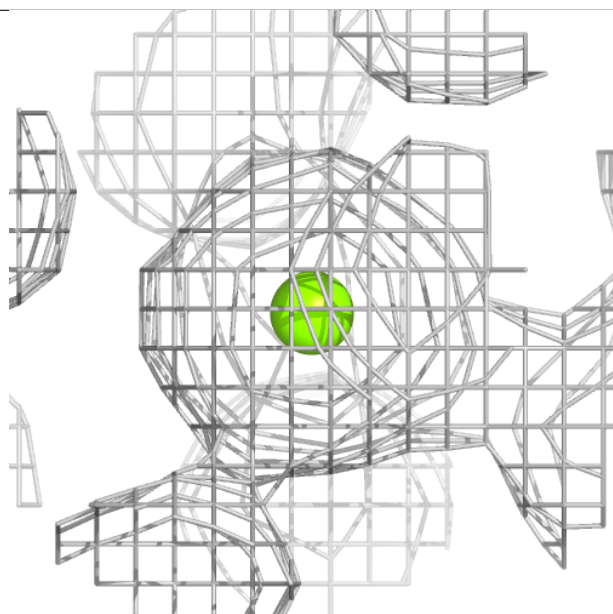
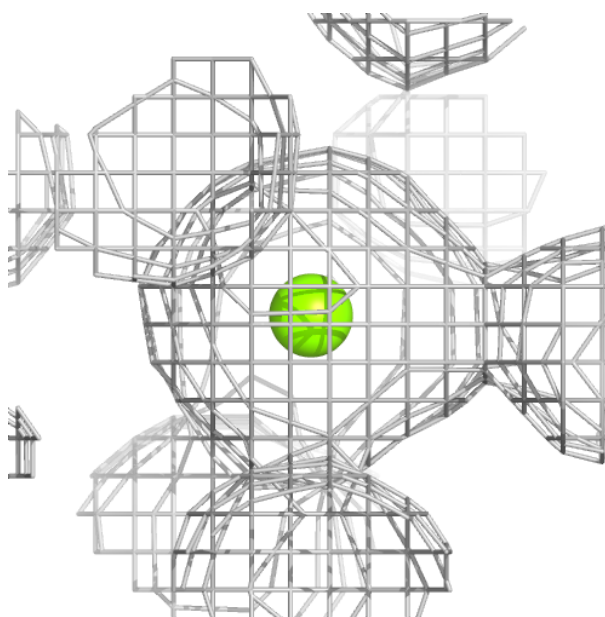
Electron density around SF4 C 303:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



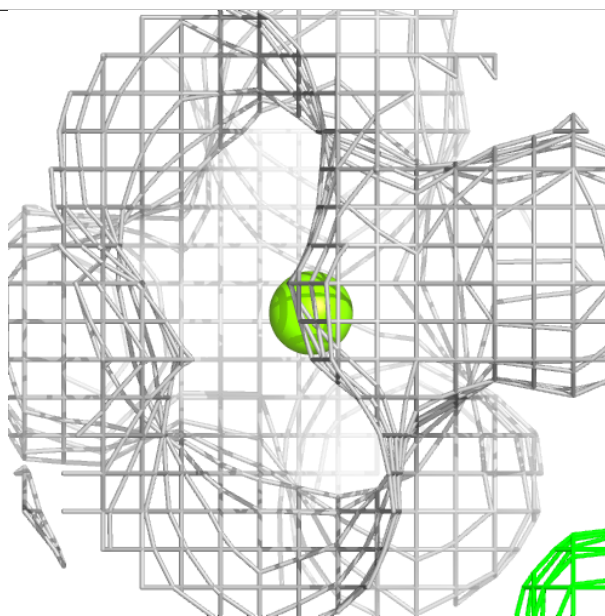
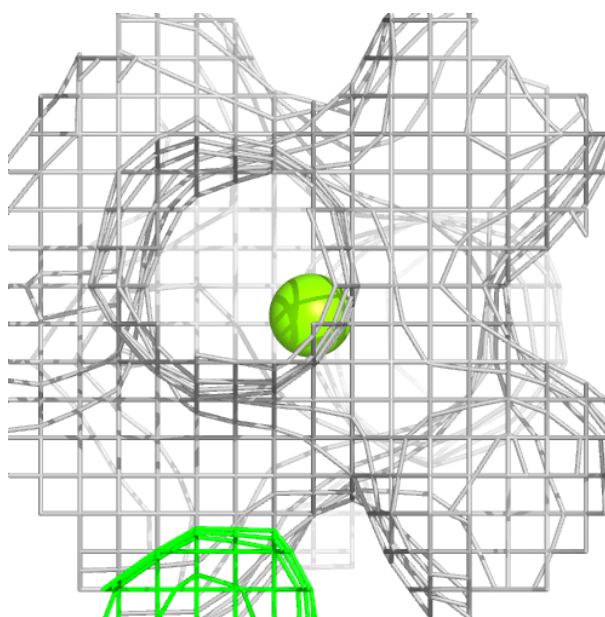
Electron density around MG N 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



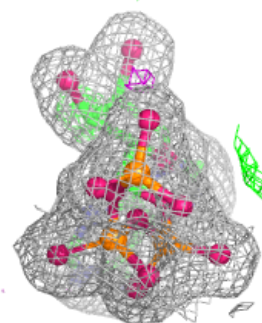
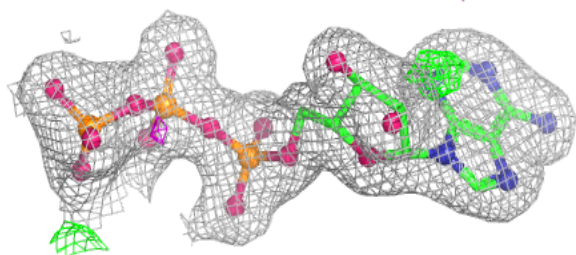
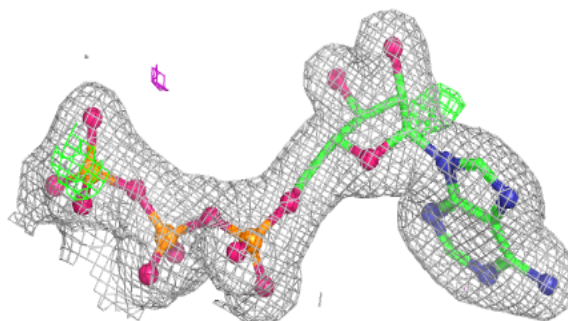
Electron density around MG O 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

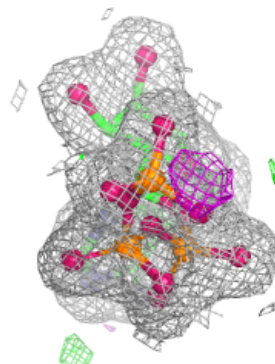
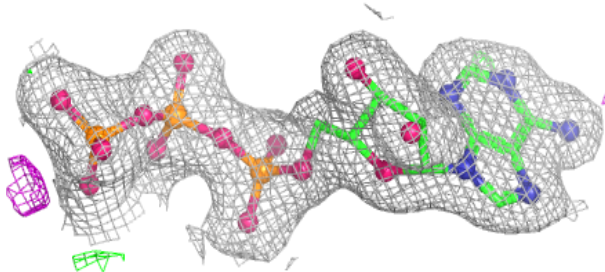
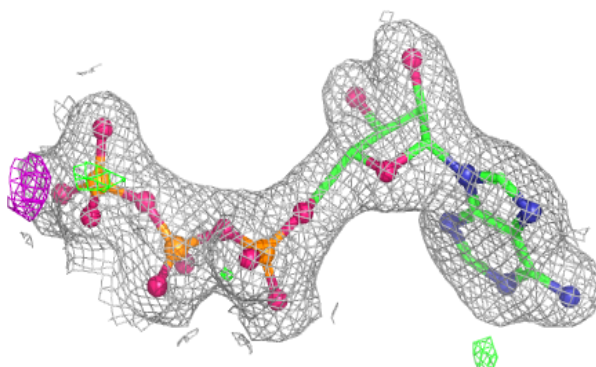


Electron density around ATP C 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

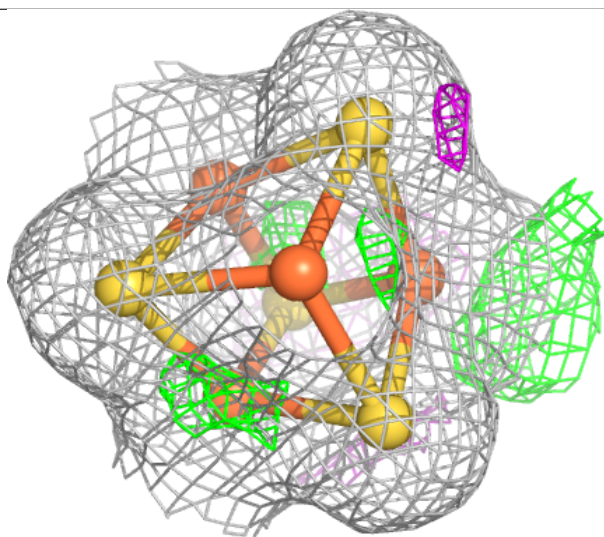
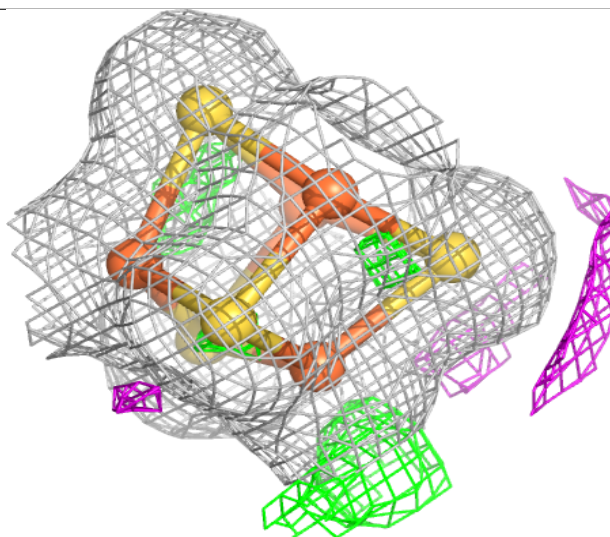
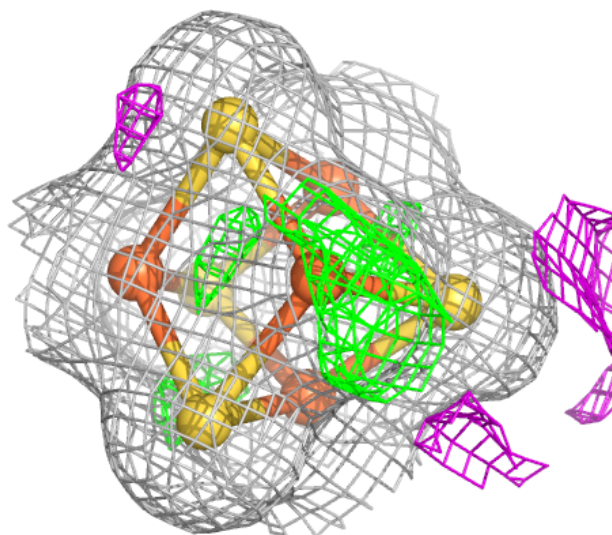
**Electron density around ATP G 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



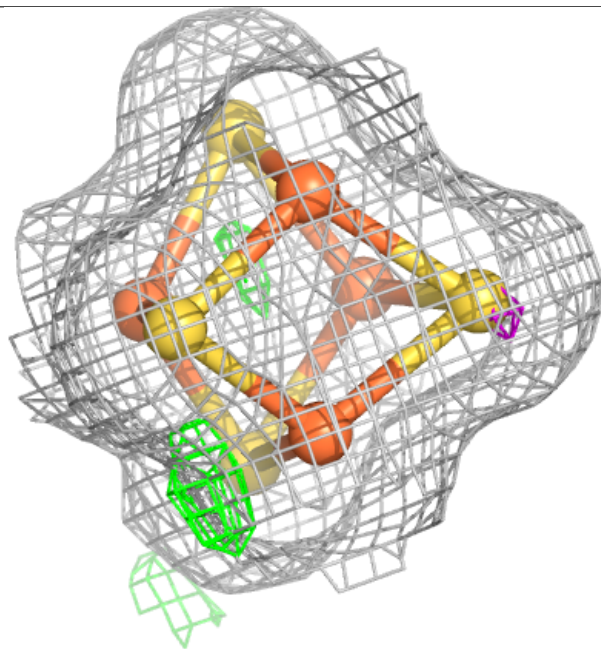
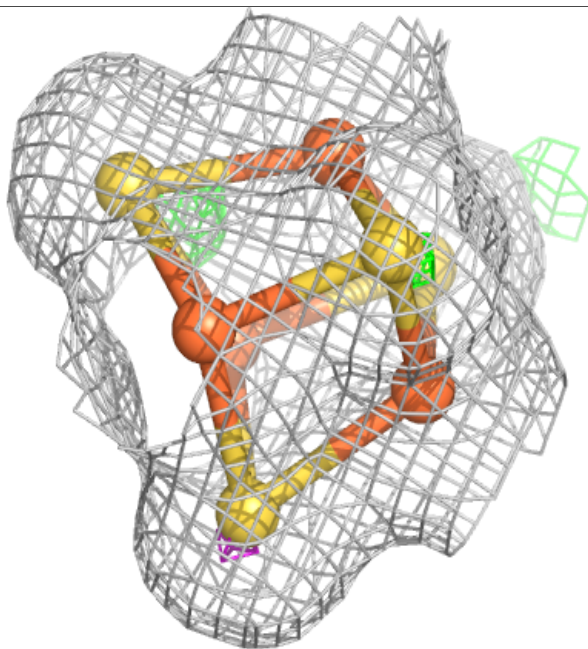
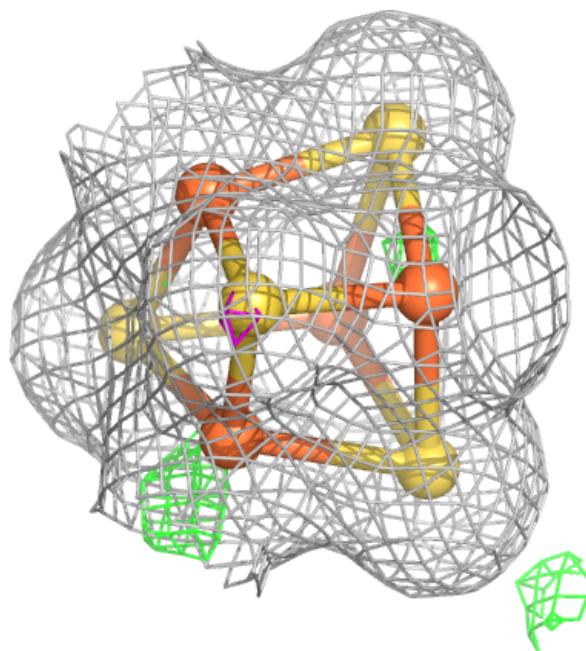
Electron density around SF4 E 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



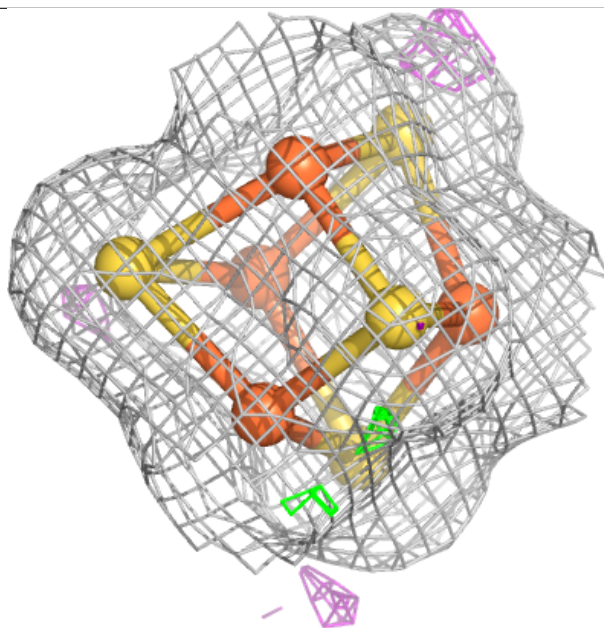
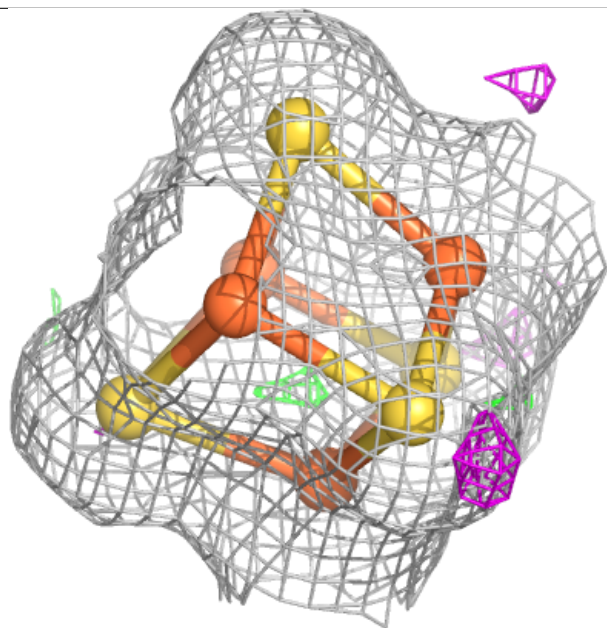
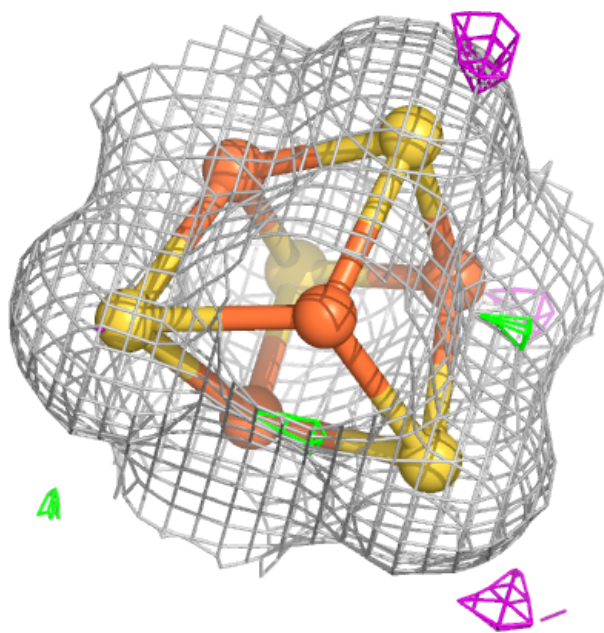
Electron density around SF4 F 401:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



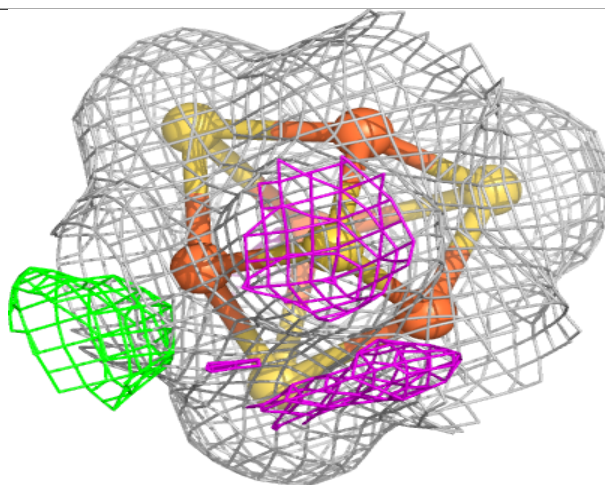
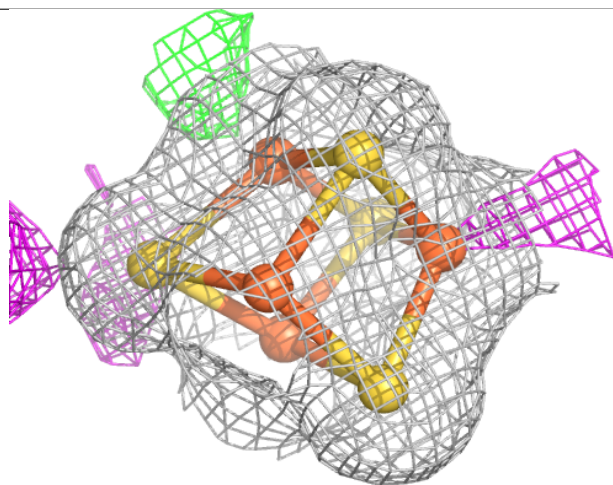
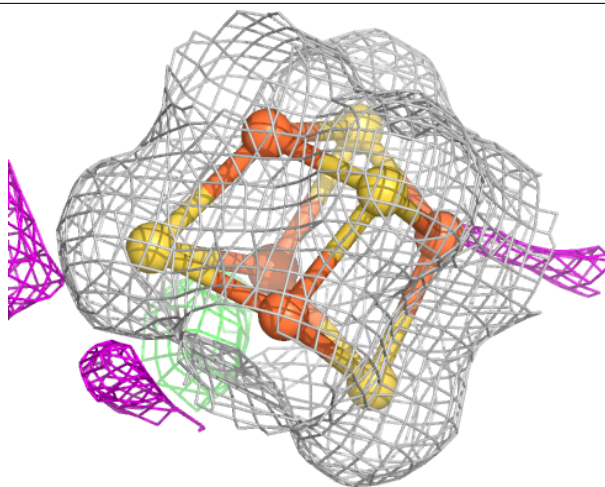
Electron density around SF4 G 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



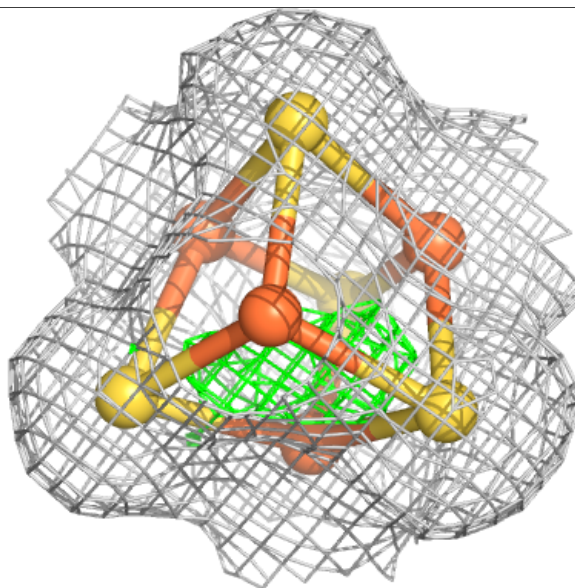
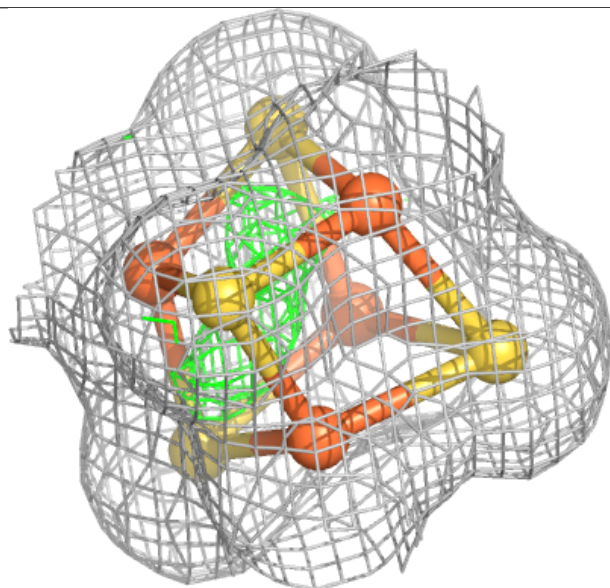
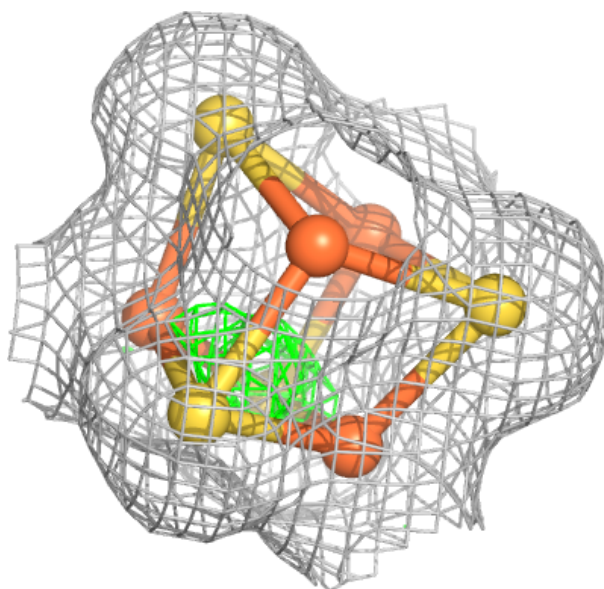
Electron density around SF4 I 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



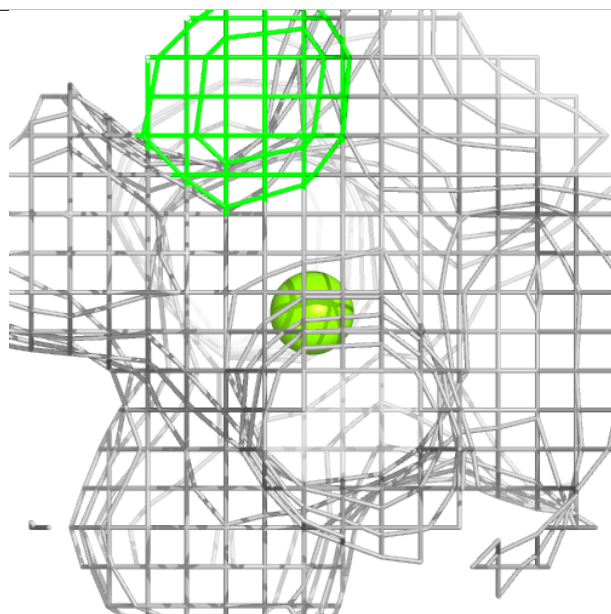
Electron density around SF4 J 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



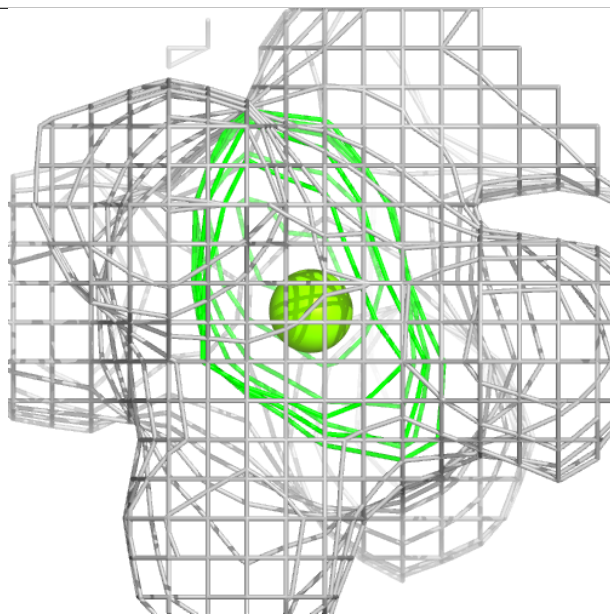
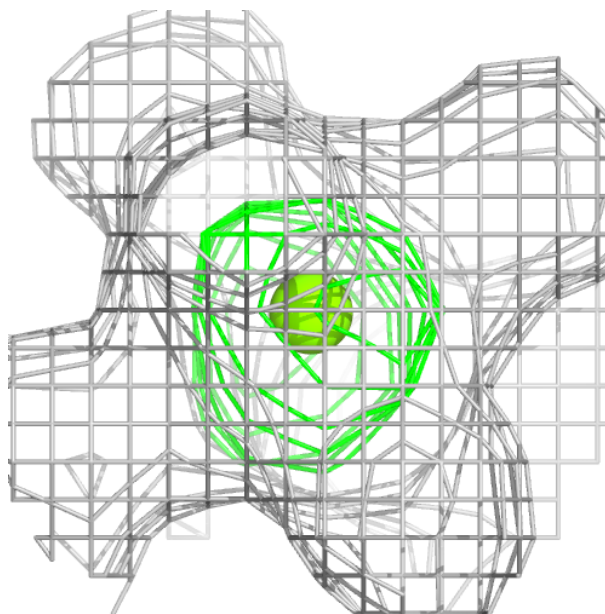
Electron density around MG K 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



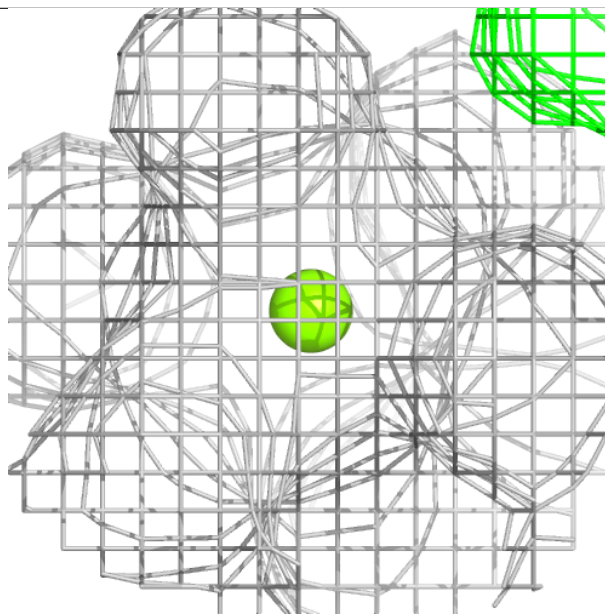
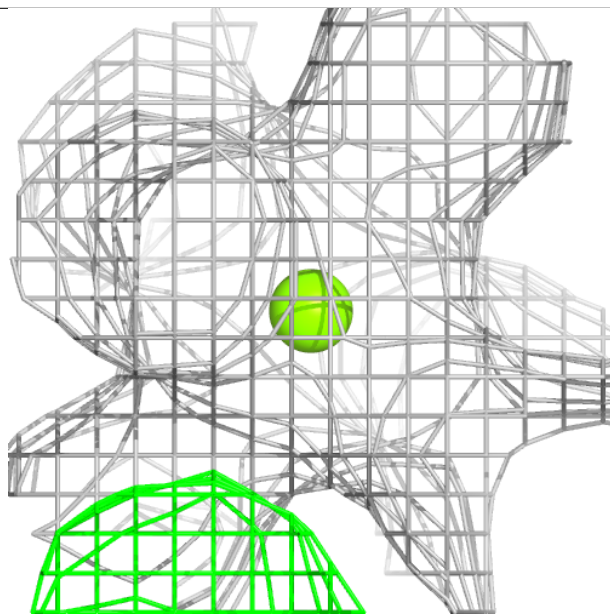
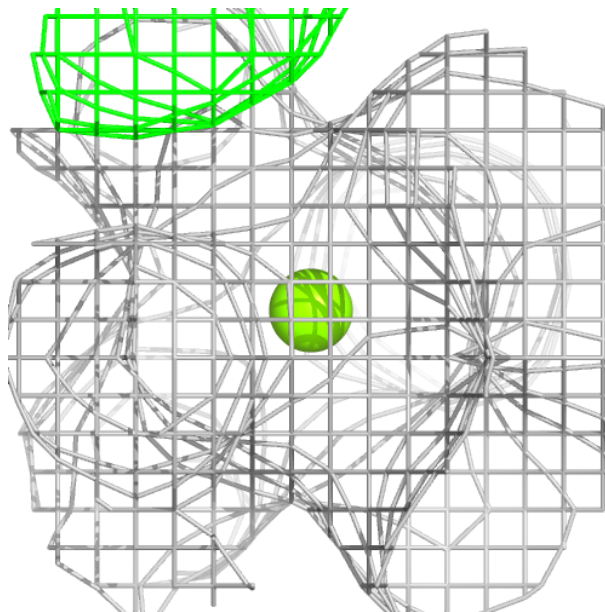
Electron density around MG L 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



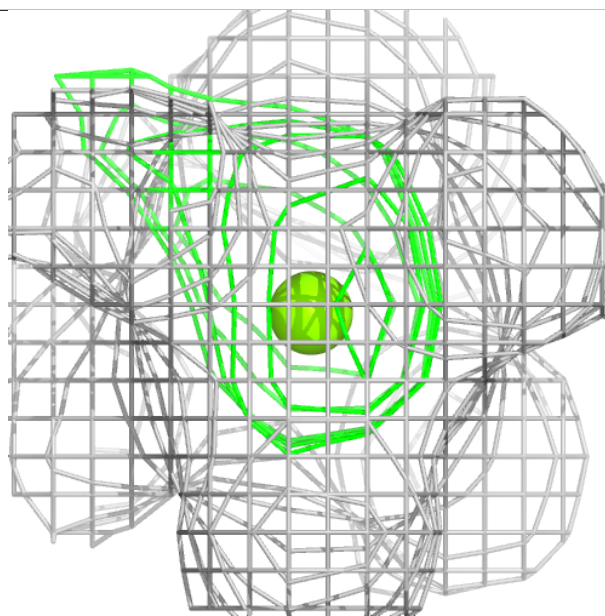
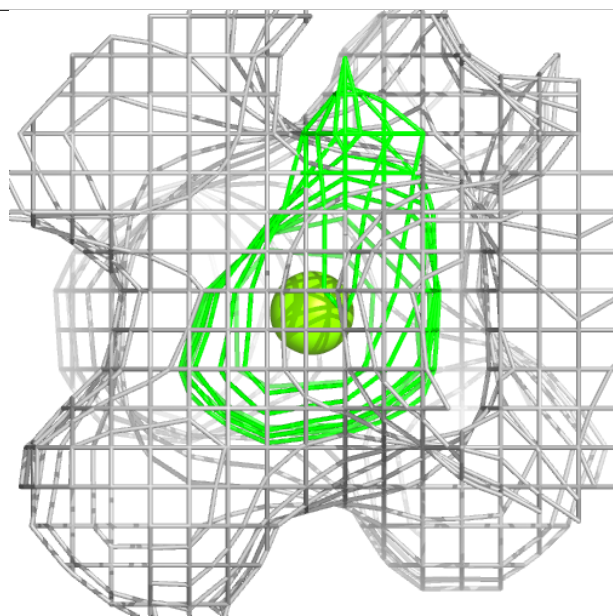
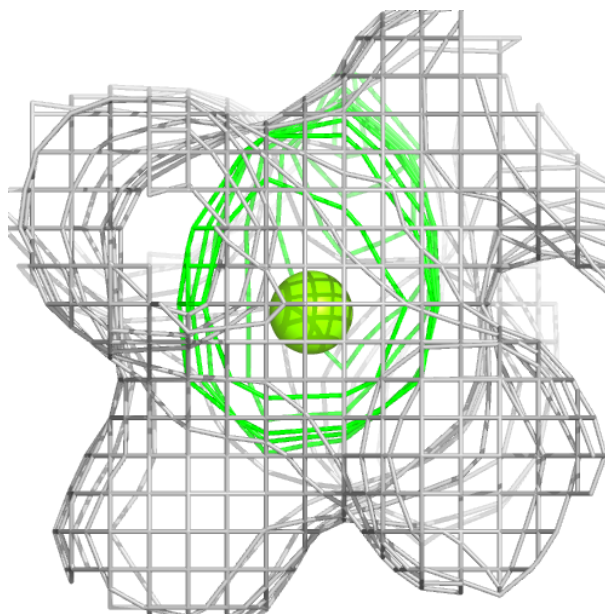
Electron density around MG C 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG P 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.